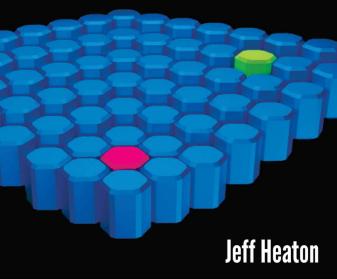
Artificial Intelligence for Humans Volume 1: Fundamental Algorithms



VISIT...



Fundamental Algorithms
Jeff Heaton
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wife, Tracy and our two cockatiels Cricket and Wynton.

This book is dedicated to my

wonderful

Introduction

- Series Introduction
- Computer Languages
- Prerequisite Knowledge
- Fundamental Algorithms
- Other Resources
- Structure of this Book

This is the first in a series of books covering select topics in Artificial Intelligence (AI). Artificial Intelligence is a large field that encompasses many sub-disciplines. The following sections introduce both the series and the first volume.

Series Introduction

This series of books introduces the reader to a variety of popular topics in Artificial Intelligence. By no means is this meant to be an exhaustive AI resource—AI is a huge field, and a great deal of information is added on a daily basis. Each book focuses on a specific area of AI.

The series teaches Artificial Intelligence concepts in a mathematically gentle manner, which is why the series is named Artificial Intelligence for Humans. Still:

- I assume the reader is proficient in at least one programming language.
 I assume the reader has a basic
- I use topics and formulas from calculus, linear algebra, differential equations, and statistics.

understanding of college algebra.

- equations, and statistics.
 However, when explaining topics in bullet point 3, I do not assume the reader is fluent in the topics
- described in the above bullet.
 I always follow concepts with realworld programming examples and pseudo code, rather than relying solely on mathematical formulas.

The target audience for this book comprises programmers who are

proficient in at least one programming language. The book's examples have been ported to a number of programming languages.

The actual book text stays at the

Programming Languages

pseudo code level. Example packs are provided for Java, C#, R, C/C++, and Python. There is also a community supplied port for the Scala programming language. Members of the community are working on porting the examples to additional languages, so your favorite language might have been ported since this printing. Check the book's GitHub repository for more information. The

other languages! If you would like to get involved, your help would be greatly appreciated. Appendix A has more information to get you started.

community is encouraged to help port to

Online Labs

Many of the examples from this series are available to run online, using HTML5. These examples use JavaScript and should run from mobile devices that are capable of HTML5.

All online lab materials can be found at the following web site:

http://www.aifh.org

These online labs allow you to try

out examples even when reading an ebook from a mobile device.

Code Repositories

All of the code for this project is released under the Apache Open Source License v2. It can be found at the following GitHub repository:

https://github.com/jeffheaton/aifh

The online labs, with Javascript Lab Examples, can be found at the following GitHub repository:

https://github.com/jeffheaton/aifh-html

Have you found something broken, misspelled, or otherwise botched? You

a commit revision to GitHub. You will be credited among the growing number of contributors. Refer to Appendix A for more information on contributing code.

Books Planned for the

probably have. Fork the project and push

Series Tunned for the

The following volumes are planned for this series:

of AIVolume 1: Fundamental Algorithms

Volume 0: Introduction to the Math

 Volume 2: Nature Inspired Algorithms

- Volume 3: Neural Networks
 Volume 4: Support Vector
- Volume 4: Support Vector Machines
- Volume 5: Probabilistic Learning

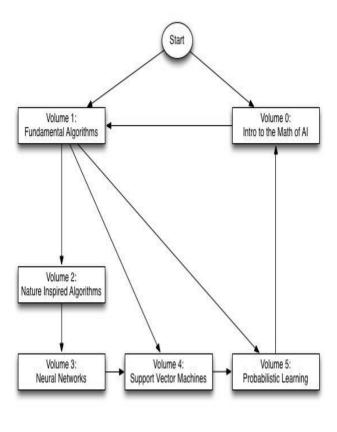
Volumes one through five will be produced in order. Volume zero is a "planned prequel" that will be produced near the end of the series to focus on the mathematical concepts introduced in the other volumes. Volumes one through five will cover required mathematical concepts, while volume zero is planned to be a recap and expansion of the mathematical concepts from the other volumes.

Volume zero can be read at either the beginning or the end of the series.

before the other volumes. Volume two does contain some information useful for volume three. Figure 1 shows the suggested reading order.

Volume one should generally be read

Figure 1: Reading the Volumes



Each volume can be read separately or as part of the series. Volume one lays down foundational algorithms that are used in each of the subsequent volumes. The algorithms of volume one are both foundational and useful in their own right.

Other Resources

There are many other resources on the Internet that will be very useful to you as you read through this series of books.

The first is the Khan Academy, which is a collection of YouTube videos that demonstrate many areas of

mathematics. If you need additional review on any mathematical concept in this book, there is most likely a video on the Khan Academy that covers it. http://www.khanacademy.org/

Second is the Neural Network FAQ. This text-only resource has a great deal of information on neural networks and other AI topics.

http://www.fags.org/fags/ai-fag/neuralnets/

The Encog wiki has a fair amount of general information on machine learning, although the information found here is not necessarily tied to Encog.

http://www.heatonresearch.com/wiki/Ma

be discussed on the Encog forums. These forums are fairly active and you are very likely to receive an answer from myself or from one of the community members at the forum. http://www.heatonresearch.com/forum

Finally, AI and neural networks can

Fundamental Algorithms Introduction

To have a great building, you must have a great foundation. This book teaches Artificial Intelligence algorithms such as dimensionality, distance metrics, clustering, error calculation, hill climbing, linear regression and discrete learning. These algorithms allow for the processing and recognition of patterns in data. This is how sites such as Amazon and NetFlix suggest products to you.

These are not just foundational algorithms for the rest of the series, but are very useful algorithms in their own right. All algorithms are explained with

numeric calculations that you can perform yourself.

Structure of this Book

Chapter one, "Introduction to AI," introduces some of the basic concepts of AI. These concepts are built upon both by this volume and the series. You will see that most AI algorithms accept an input array of numbers and produce an output array. Problems to be solved by AI are often modeled to this form. Internally, the algorithm keeps additional arrays that effectively represent long and short-term memory. These algorithms are trained by adjusting the long-term memory to produce a desirable output for a given input.

Chapter two, "Normalizing Data,"

prepared for many AI algorithms. Data is presented to an algorithm in the form of an input array. Not all data is numeric and some is categorical. Examples of categorical data include color, shape, gender, species, and any other nonnumeric descriptive quality. Numeric data must often be normalized to a specific range. Numeric qualities are often normalized to a range between -1 and 1.

shows how raw data is typically

Chapter three, "Distance Metrics," shows how data can be compared in much the same way as we plot a distance between two points on a map. AI often works with numeric arrays. These arrays hold input data, output data, long-term

information. These arrays are often called vectors. We can calculate the distances between these data points in much the same way as we calculate the distance between two points. Two-

memory, short-term memory, and other

dimensional and three-dimensional points can be thought of as vectors of length two and three, respectively. In AI, we often deal with spaces of much higher dimensionality than three.

Chapter four, "Random Numbers,"

shows how random numbers are calculated and used by AI algorithms. This chapter begins by discussing the difference between uniform and normal

random numbers. Sometimes AI algorithms call for each random number

times, random numbers must follow a distribution. The chapter additionally discusses techniques for random number generation.

to have an equal probability. At other

Chapter five, "K-Means Clustering," shows how data can be grouped into similar clusters. K-Means is an algorithm can be used by itself to group data into groups by commonality. Additionally, K-Means is often used as a component to other more complex algorithms. Genetic algorithms often use K-Means to group populations into species with similar traits, while online retailers often use clustering algorithms to break customers into clusters. Sales suggestions can then be created based on the buying habits of members of the same cluster.

Chapter six, "Error Calculation,"

shows how the results of AI algorithms

can be evaluated. Error calculation is how we determine the effectiveness of an algorithm, which can be done using a scoring function that evaluates the effectiveness of a trained algorithm. A very common type of scoring function simply contains input vectors and expected output vectors. This is called training data. The algorithm is rated based on the distance between the algorithm's actual output and the

Chapter seven, "Towards Machine Learning," introduces simple algorithms

expected output.

that can be trained to analyze data and produce better results. Most AI algorithms use a vector of weighted values to transform the input vector into a desired output vector. This vector of weighted values forms a sort of longterm memory for the algorithm. Training is the process of adjusting this memory to produce the desired output. This chapter shows how to construct several simple models that can be trained and introduces relatively simple, yet effective, training algorithms that can adjust this memory to provide better output values. Simple random walks and hill climbing are two such means for

setting these weights. Chapter eight, "Optimization introduced in the previous chapter. These algorithms, which include Simulated Annealing and Nelder Mead, can be used to quickly optimize the

Algorithms," expands the algorithms

weights of an AI model. This chapter shows how to adapt these optimization algorithms to some of the models introduced in the previous chapter.

Chapter nine, "Discrete Optimization," shows how to optimize data that is categorical rather than numeric. Not every optimization problem is numeric, as we see in the cases of discrete, or categorical, problems such as the Knapsack Problem

and the Traveling Salesman Problem. This chapter shows that Simulated these two problems. Simulated annealing can be used for continuous numeric problems and discrete categorical problems.

Chapter ten, "Linear Regression,"

Annealing can be adapted to either of

Chapter ten, "Linear Regression," shows how linear and non-linear equations can be used to learn trends and make predictions. The chapter introduces simple linear regression and shows how to use it to fit data to a linear model. This chapter will also introduce the General Linear Model (GLM), which

can be used to fit non-linear data.

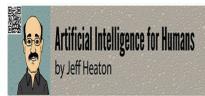
The Kickstarter Campaign

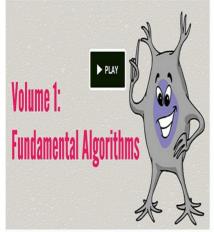
in 2013 as the result of a successful Kickstarter campaign. The home page for the Kickstarter project is shown in Figure 2.

This series of books was launched

Figure 2: The Kickstarter Campaign

Funded! This project successfully raised its funding goal on Jul 10.





818

pledged of \$2,500 goal

seconds to go

Funding period

Jun 10, 2013 - Jul 10, 2013 (30 days)



Project by Jeff Heaton St. Louis, MO

Contact me

First created - 8 backed

Kickstarter at the following link: http://goo.gl/dGorA

You can visit the original

I would like to thank all of the

Without your support, this series might not exist. I would also like to extend a special thanks to those backers who supported at the \$100 and higher levels.

Kickstarter backers of the project!

They are listed here, in order that they pledged.

Figure 3: Kickstarter 100 Dollar Level Supporters

Dr. Warren D. Lerner Dave Snell Ovvind R Lorentzen Jeffrey Elrod Anders Steffen Öding Andersen Rick Cardarelle Andy Eunson Tracy Turnage Heaton Davíð Helgason Patrick Saint - laurent Bradford Nazario Barr Chris Duesing Arsham Hatambeiki Alex Brem Randy J. Ray Matthew Schissler Matthew March Yvonne Norton Leung Travis Thaxton

the project to the \$2,500 minimum requested amount. A very big thank you to Rory Graves and Matic Potocnik porting the examples to Scala.

Cardarelle! His pledge of \$358 pushed

Also a big thanks to Rick

Thank you everyone—you are the best!

Chapter 1: Introduction to AI

- Relationship to Human Brains
- Modeling Input and Output
- Classification and Regression
- Time Series
- Training

Most laypeople think of Artificial Intelligence (AI) as a sort of artificial brain and recall images from science fiction movies about robots. Such images have very little to do with how AI is actually used in today's world. It is true that AI has many similarities to

human brain function, but the significant distinction is that Artificial Intelligence is artificial. AI does not need to pretend to be biological.

Before we get too deep, I would

like to introduce some very general concepts about how you interact with an AI algorithm. The AI algorithm is the technique that you are using to solve a

problem. An AI algorithm is sometimes called a model. There are many different AI algorithms, or models. Some of the most common are Neural Networks, Support Vector Machines, Bayesian

Support Vector Machines, Bayesian networks, and Hidden Markov Models. This series of books covers many of these models.

It is important for the AI

a problem to an AI program, as this is the primary mode of interaction with an AI algorithm. We will begin our foundation of knowledge in this topic by exploring how the human brain interacts with its world.

practitioner understand how to represent

Relationship to Human Brains

The purpose of AI is to allow a

computer to function somewhat like a human brain. However, this does not mean that AI seeks to emulate every aspect of the human brain. The degree to which an AI algorithm matches the actual functioning of the human brain is called biological plausibility.

Christof Koch, chief scientific officer of the Allen Institute for Brain Science, calls the brain "the most complex object in the known universe." (Koch, 2013) In the context of AI, the brain is essentially an advanced piece of

technology that we must study, reverse engineer, and learn to emulate.

The brain is not the only piece of

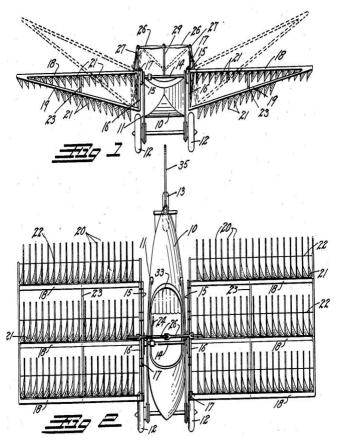
"advanced technology" that nature has

shared with us. Flight is another. Early airplanes attempted to emulate the flapping wings of birds. Such airships are called ornithopters. These flapping

airships did not work very well, however. Figure 1.1 shows a patent

diagram for the Gray Goose Ornithopter.

Figure 1.1: Gray Goose Ornithopter
(US patent 1,730,758)



Biological birds were the only models for flying machines in existence through the early 1900s. It seemed logical to emulate birds, as they were excellent flyers. However, from experimenting with flying machines, humans have learned not to follow the path of nature too closely. While we wanted to emulate the end goal of flying, emulating exactly how natural bird flight occurs did not result in an effective flying machine.

The abstraction of emulation occurs in many other contexts. My MacBook Pro can emulate a Windows PC, and can also emulate a Commodore 64. A C64 is somewhat different from my more modern laptop, in more than just looks.

computers. When my Mac emulates a C64, it does not emulate the actual transistors that make up a C64's 6510 microprocessor. The emulation occurs at a higher level. This is the same in AI. Some algorithms emulate neurons, while some, like my C64 emulator, operate at a higher level. We focus on the end goal of providing functionality in a PC context, rather than directly emulating all the processes that lead to functionality in a brain.

What you want to do is more

important than how. At the highest level, there are similarities between a human

The instruction set that drives a C64 is quite different from the Intel x86 instruction set common on many modern

brain and most AI algorithms. The next section will examine these.

The Brain and Its World

Before we begin, let's look at how the human brain works on an external level. While we know relatively little about the internal operation of the brain, we do know a fair amount about the external operation of the brain.

The brain is essentially a black box connected by nerves. These nerves carry signals between the brain and the body. A certain set of inputs causes a certain output. For example, feeling your finger about to touch a hot stove will result in

other nerves sending commands to your muscles to pull your finger back.

It is also very important to note that the brain has an internal state. Consider

if you suddenly heard a horn. How you react is determined not just by the

stimuli of the horn, but where you are when you hear the horn. Hearing a horn in the middle of a movie evokes a very different response than hearing a horn when you are crossing a busy street. The knowledge of where you are creates a certain internal state that causes your brain to react differently to different contexts. The order in which stimuli are

received is also important. A common game is to close your eyes and attempt to

your fingers over it. As your fingers run over the object, you receive information that forms an image of what the object is.

You can essentially think of the human brain as a black box with a series of inputs and outputs. Our nerves

provide our entire perception of the world. The nerves are the inputs to the brain. There is actually a finite number

use only touch to determine what an object is. When you grab the object, you

information to determine what it is. Rather, you must grab the object and run

not instantly receive enough

of inputs to a typical human brain.

Likewise, our only means to interact with the world are the outputs from our nerves to our muscles. The

of the inputs and internal state of the brain. In response to any input, the human brain will alter its internal state and produce output. The significance of the order of the inputs is handled by the internal state of the brain.

output from the human brain is a function

Brain in a Vat

is the inputs we receive from sensory inputs and out actions through motor nerves, what actually is "reality"? Your brain is hooked up to your body, but it could also be hooked up to a simulation, as in the movie, The Matrix. So long as the output from your brain is producing

If our only interaction with reality

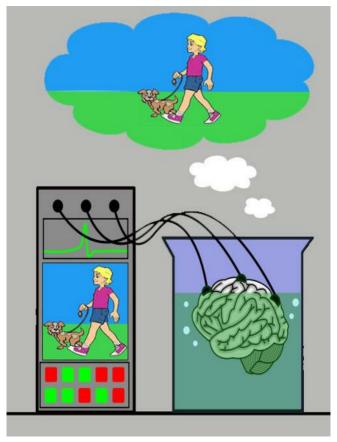
the expected inputs, would you know what was real and what was simulated? This is a common philosophical

thought experiment called "brain in a

vat." Figure 1.2 illustrates the brain in a vat thought experiment. In the figure, the brain believes that its body is walking a dog. But does the brain have a body? Does the dog even exist? What does

"exist" even mean? All we really know is what our nerves tell us. (Sigiel, 1999)

Figure 1.2: Brain in a Vat



Nerves would be connected to a supercomputer that would provide electrical impulses identical to those the brain normally receives. The computer would then be simulating reality by including appropriate responses to the

brain's output. The disembodied brain would continue to have perfectly normal

person's brain could be removed from the body and provided life-support.

This experiment assumes that a

conscious experiences outside of the "real world." There are even philosophical theories that suggest we are living in a simulation. (Bostrom, 2003)

One attempt to model an algorithm directly from the human brain is the

small part of AI research, and the neural network model aligns very closely with many of the AI algorithms that you will learn in this series of books.

Computer based neural networks

neural network. Neural networks are one

are not like the human brain in that they are not general-purpose computation devices. Neural networks, as they currently exist, carry out very small, specific tasks. An AI algorithm experiences its reality by providing output based on the algorithm's internal state and the input it is currently receiving. The "reality" that the algorithm is attached to may change as the researcher experiments with the algorithm.

This model of inputs, outputs, and internal state holds true for most AI algorithms, regardless of whether you are creating AI for a robot or a stock picker. Of course, some algorithms are more complex than others.

Modeling Problems

Knowing how to model a real-world problem to a machine-learning algorithm is critical. Different problems will lend themselves to different algorithms. At the highest level, you will model your problem in one of four different ways:

- Data classification
- Regression analysis
- Clustering
- Time Series

Sometimes you will model one problem using several of these

approaches. We will examine each of these, beginning with data classification.

Data Classification

Classification attempts to determine the class in which the input data falls into. Classification is usually a supervised training operation, which occurs when the user provides data and expected results to the machine-learning algorithm. In data classification, the expected result is identification of the data class.

Supervised training always deals with known data. During training, machine-learning algorithms are

classify known data. The hope is that the algorithm, once trained, will be able to classify unknown data as well.

Fisher's Iris Dataset is an example

of classification. (Fisher, 1936) This

evaluated according to how well they

dataset contains measurements of iris flowers. This is one of the most famous datasets and is often used to evaluate machine-learning algorithms. The full dataset is available at the following URL:

http://www.heatonresearch.com/wiki/Iris

Below is a small sampling from the

iris dataset.

"Sepal Length", "Sepal Width", "Pet 5.1, 3.5, 1.4, 0.2, "setosa"

```
4.7,3.2,1.3,0.2,"setosa"
...
7.0,3.2,4.7,1.4,"versicolor"
6.4,3.2,4.5,1.5,"versicolor"
6.9,3.1,4.9,1.5,"versicolor"
...
6.3,3.3,6.0,2.5,"virginica"
5.8,2.7,5.1,1.9,"virginica"
```

7.1,3.0,5.9,2.1, "virginica"

4.9,3.0,1.4,0.2, "setosa"

The above data are shown as a CSV file. CSV is a very common input format for machine learning. The first row is typically a definition for each of the columns in the file. As you can see, for each of the flowers there are five pieces of information provided:

Sepal length

- Sepal widthPetal length
- Petal width
- Species

For classification, the algorithm is instructed to determine the species of the flower given the sepal length/width and the petal length/width. The species is the class.

A class is usually a non-numeric

data attribute and, as such, membership in the class must be well defined. For the Iris dataset, there are three different types of iris. If a machine-learning algorithm is trained on three types of iris, it cannot be expected to identify a rose. All members of the class must be known at the time of training.

Regression Analysis

In the last section, we learned how to use data to classify data. But often the desired output is not simply a class, but a number. Consider the calculation of an automobile's fuel efficiency in miles per gallon (MPG). Provided data such as the engine size and car weight, the MPG for the specified car may be calculated.

The following sample provides MPG data for five cars:

```
"mpg", "cylinders", "displacement", 18.0,8,307.0,130.0,3504.,12.0,70, 15.0,8,350.0,165.0,3693.,11.5,70,
```

18.0,8,318.0,150.0,3436.,11.0,70, 16.0,8,304.0,150.0,3433.,12.0,70, 17.0,8,302.0,140.0,3449.,10.5,70, ...

found at the link below: (Quinlan, 1993)
http://www.heatonresearch.com/wiki/MI
A regression analysis aims to train

The entirety of this dataset may be

the algorithm with input data about the car to provide an answer calculated from input. In this case, the algorithm would be asked to determine the miles per gallon that the specified car would likely get.

It is also important to note that not every piece of data in the above file will be used. The columns "car name" and has nothing to do with its fuel efficiency and is therefore excluded from the calculation. Likewise, the origin of the car does not contribute to this equation. Although the origin is given a numeric value that specifies what geographic region the car was produced in and some regions do focus more on fuel efficiency than others, this piece of data is far too broad to be useful.

"origin" are not used. The name of a car

Clustering

Clustering is very similar to classification in that the computer is required to group data. Clustering algorithms take input data and place it

specifies the number of clusters to be created before training the algorithm. The computer places similar items together using the input data. Because you do not specify what cluster you expect a given item to fall into, clustering is useful when you have no expected output. Because there is no expected output, clustering is considered unsupervised training.

into clusters. The programmer usually

Consider the car data from the previous section. You might run a clustering algorithm to break the cars into four groups. This would tell you what cars are similar to each other.

The difference between clustering

the algorithm the freedom to find order in the data. Classification teaches the algorithm what class known data should fit into, with the goal of allowing the trained algorithm to eventually classify new data that the algorithm was not trained with.

and classification is that clustering gives

Clustering and classification algorithms handle new data differently. The entire purpose of classification is to be able to classify new data based on previous data with which the algorithm was trained, while clustering makes no provision for new data. If you want to add new data to the existing groups, you must reclassify the entire data set.

Time Series

Machine learning algorithms work somewhat like mathematical functions. They map the input values to output values. If there is no internal state to the machine-learning algorithm, a given set of inputs will always produce the same outputs. Many machine-learning methods do not have an internal state that changes and affects the output. For example, in the context of the car data, you would want the classification algorithm's decision to be supported by all the data, rather than just by the last few cars that it has seen.

Time series is often very important.

do not care about time series. However, if your only input is the current price of a stock, time series becomes very important. A single price point for a stock on a given day does not help much for prediction. However, a trend considering several days of stock prices may be of use.

Some machine-learning algorithms support it and others do not. If you are classifying cars or irises you most likely

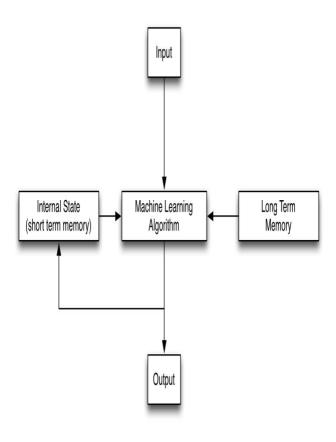
There are also methods to encode time series into algorithms that do not directly support time series. In these cases you make the previous days part of the input. For example, you may have five inputs that represent the previous five days of trading from the day you



Modeling Input and Output

Earlier in this chapter I mentioned that a machine-learning algorithm is provided with input and produces output. This output is affected by the algorithm's long- and short-term memory. Figure 1.3 shows how long- and short-term memory are involved in the output process.

Figure 1.3: Abstract Machine Learning Algorithm



output. Most machine learning algorithms operate completely synchronously. The algorithm will only output when presented with input. It is not like a human brain, which always responds to input but occasionally produces output without input!

So far we have only referred to the

above accepts input and produces

As you can see, the algorithm

input and output patterns abstractly. You may be wondering exactly what they are. The input and output patterns are both vectors. A vector is essentially an array of floating point numbers, as shown below:

Input: [-0.245, .283, 0.0]

algorithms have a fixed number of inputs and outputs. They work like functions in computer programs. The input can be thought of as the parameters to a function. The output is the return value. For the above data an algorithm would accept three input values and return two output values. These counts do not typically change. As a result, the number of elements in the input and output patterns for a particular algorithm can never change.

Nearly all machine learning

To make use of the algorithm, you must express your problem in such a way as to have the input to the problem

Likewise, the solution to the problem must be an array of floating point numbers. This is really all that most algorithms can do for you. Machine learning algorithms take one array and

be an array of floating point numbers.

transform it into a second. Many pattern recognition algorithms are something like a hash table in traditional programming. In traditional programming, a hash table is used to map keys to values. In many ways, a hash table is somewhat like a dictionary, in that it includes a term and its meaning. A hash table could look like the following:

- "hear" -> "to perceive or apprehend by the ear"
 "run" -> "to go faster than a walk"
- "write" -> "to form (as characters or symbols) on a surface with an instrument (as a rank)"

instrument (as a pen)"

The above example is a mapping

between words and their definitions.

This hash table uses a key of string and applies it to another value of a string. If you provide the dictionary with a key (the word), it returns a value (the definition). This is how most machine learning algorithms function.

All program hash tables use keys and values. Think of the pattern sent to the input layer of the algorithm as the key value returned from the hash table as the pattern that is returned from the output layer of the algorithm. Of course, an algorithm is much more than a simple hash table.

to the hash table. Likewise, think of the

With the above hash table, what would happen if you were to pass in a word that is not a key in the map? For example, the key "wrote." A hash table would return null or in some way indicate that it could not find the specified key. Machine learning algorithms, on the other hand, do not return null. They find the closest match,

or a probability of a match. If you passed "wrote" to the algorithm above,

you would likely get back what you

Not only does the algorithm find the closest match, it will modify the output

would have expected for "write."

to guess the missing value. Of course, there is not enough data for the algorithm to have modified the response in the example above, as there are only three

samples. When the data is limited the

closest match may not be very meaningful.

The above mapping brings up one very important point about these algorithms. Given that algorithms accept an array of floating point numbers and return another array, how would you put

strings into the algorithm? There is a way to do this, although it is much easier to deal with numeric data than strings.

(Harris, 1954) Each input represents the count of one particular word. The entire input vector would contain one value for each unique word. Consider the following strings.

common means of encoding strings.

The Bag of Words algorithm is a

Mice and More Mice

We have the following unique

words. This is our "dictionary."

Input 0: and
Input 1: blind
Input 2: bluff

Input 3: man's
Input 4: men

Of Mice and Men
Three Blind Mice
Blind Man's Bluff

Input 6: more
Input 7: of
Input 8: three

Input 5: mice

The four lines above would be encoded as follows.

Of Mice and Men [0 4 5 7] Three Blind Mice [1 5 8] Blind Man's Bluff [1 2 3] Mice and More Mice [0 5 6]

Of course we have to fill in the missing words with zero, so we end up with the following.

Of Mice and Men [1, 0, 0, 0, 1, 1]
Three Blind Mice [0, 1, 0, 0, 0,
Blind Man's Bluff [0, 1, 1, 1, 0,
Mice and More Mice [1, 0, 0, 0, 0, 0]

the total number of words in our "dictionary". Each component number in the vector is an index into our dictionary of available words. At each vector component is stored a count of the number of words for that dictionary entry. Each string will usually contain only a small subset of the dictionary. As a result, most of the vector values will be zero.

Notice that we now have a

consistent vector length of nine. Nine is

As you can see, one of the most difficult aspects of machine learning programming is translating your problem into a fixed-length array of floating point numbers. The following section shows how to translate several examples.

A Simple Example

If you have read anything about machine learning, you have no doubt seen examples with the **XOR** operator. A program learning the **XOR** operator is essentially the "Hello World" of AI. This book will describe scenarios much more complex than XOR, but the XOR operator is a great introduction. We shall begin by looking at the XOR operator as though it were a hash table. If you are not familiar with the **XOR** operator, it works similarly to the AND and **OR** operators in that it considers two sides and generates a true or false answer. An AND operator is true when both sides are true. Likewise an **OR** is

For an **XOR** to be **true**, both of the

sides must be different from each other. The truth table for an **XOR** is as follows.

```
False XOR False = False
True XOR False = True
False XOR True = True
True XOR True = False
```

The above truth table would be represented in hash table form as follows:

```
[ 0.0 , 0.0 ] -> [ 0.0 ] [ 1.0 , 0.0 ] -> [ 1.0 ] [ 0.0 , 1.0 ] -> [ 1.0 ] [ 1.0 , 1.0 ] -> [ 0.0 ]
```

These mappings show the input and the ideal expected output for the algorithm.

Miles per Gallon

Machine learning problems usually involve dealing with a set of data and using a calculation to predict the output data or to determine a course of action. Consider a car database that contains the following fields:

- Car weight
- Engine displacement
- Cylinder count
- Horse power

- Hybrid or gasoline
- Miles per gallon

Assuming you have collected some data for these fields, you should be able to construct a model that can predict one field value based on the other field values. For this example, we will try to predict miles per gallon.

We will need to define this

problem in terms of an input array of floating point values mapped to an output array of floating point values. Furthermore, the numeric range on each of these array elements should be between 0 and 1 or -1 and 1. This is called normalization. Normalization will be covered in much greater detail in the

next chapter.

First, we see how we would

normalize data from above. Consider the input and output data formats. We have six total fields. We want to use five of these to predict the sixth. The algorithm would have five inputs and one output.

Your algorithm's input and output would look something like the following.

- Input 1: Car weight
- Input 2: Engine displacement
 - Input 3: Cylinder count
- Input 4: Horse power
- Input 5: Hybrid or gasoline
- Output 1: Miles per gallon

To do this we must think of reasonable ranges for each of these values. We will then transform input data into a number between 0 and 1 that represents an actual

We also need to normalize the data.

value's position within that range. The following example establishes reasonable ranges for these values:

- Car weight: 100–5000 lbs
 Engine displacement: 0.1–10 liters
- Cylinder count: 2–12
- Horse power: 1–1000
- Hybrid or gasoline: true or false
- Miles per gallon: 1–500

These ranges may be a little large for modern cars. However, this will

use ranges that will not invite too much data at their extreme ends, so a large range is best.

We will now look at an example.

allow minimal restructuring to the algorithm in the future. It is also best to

How would we normalize a weight of 2,000 pounds? This weight is 1,900 into the range and the size of the range is 4,900 pounds. The percent of the range

size is 0.38 (1,900 / 4,900). Therefore, we would feed the value of 0.38 to the algorithm input to represent this value. This satisfies the typical range requirement of 0 to 1 for an input.

The hybrid or regular value is a true/false. To represent this value we will use 1 for hybrid and 0 for regular.

We simply normalize a true/false into two values.

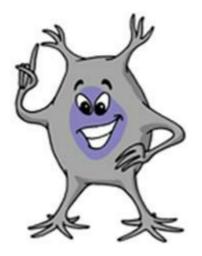
Presenting Images to Algorithms

Images are a popular source of input for algorithms. In this section, we will see how to normalize an image. There are more advanced methods than this, but this method is often effective.

Consider a full-color image of 300x300 pixels. 90,000 pixels times the three RGB colors gives 270,000 total pixels. If we had an input for each pixel, that would be 270,000 inputs. This is just too large for many algorithms.

Thus, we need to downsample. Consider the following image, which is at full resolution (Figure 1.4).

Figure 1.4: An Image at Full Resolution



We will now downsample it to 32x32, as shown below (Figure 1.5).

Figure 1.5: An Image Downsampled



The grid-like pattern of the image after it has been reduced to 32x32 pixels

input to an algorithm. This algorithm would require 1,024 inputs, if the algorithm were to only look at the intensity of each square. Looking at the intensity causes the algorithm to "see" in black and white.

allows us to use the pixels to form the

If you would like the algorithm to see in color, then it is necessary to provide the intensity of red, green, and blue (RGB) values for each of these pixels. This would mean three inputs for each pixel, which would push our input count to 3,072.

The normal intensity range for RGB values is between 0 and 255. To create input for the algorithm, simply divide the intensity by 255 to create an intensity

percentage. For example, intensity number 10 becomes 10/255, or 0.039.

You may be wondering how the

outputs will be handled. In a case such as this, the outputs should communicate what image the algorithm believes it is looking at. The usual solution is to create one output for each type of image

the algorithm should recognize. The algorithm will be trained to return a value of 1.0 for the output that corresponds to what the image is believed to be.

We will continue showing you how to format algorithms for real-world problems in the next section, which will

take a look at financial algorithms.

Financial Algorithms

Financial forecasting is a very popular form of temporal algorithm. A temporal algorithm is one that accepts input for values that range over time. If the algorithm supports short term memory (internal state) then ranges over time are supported automatically. If your algorithm does not have an internal state then you should use an input window and a prediction window. Most algorithms do not have an internal state. To see how to use these windows, consider if you would like the algorithm to predict the stock market. You begin with the closing price for a stock over several days.

Day 4: \$40 Day 5: \$41 Day 6: \$43 Day 7: \$45 Day 8: \$57 Day 9: \$50 Day 10:\$41 The first step is to normalize the data. This is necessary whether your algorithm has internal state or not. To normalize, we want to change each number into the percent movement from

Day 1: \$45 Day 2: \$47 Day 3: \$48

would become 0.04, because there is a 4% difference between \$45 and \$47. Once you perform this calculation for every day, the data set will look like the

the previous day. For example, day 2

Day 2: 0.04 Day 3: 0.02

following:

Day 4:-0.16 Day 5: 0.02

Day 6: 0.04 Day 7: 0.04

Day 8: 0.04 Day 9:-0.12

Day 10:-0.18

will predict the next day's values, we need to think about how to encode this data to be presented to the algorithm. The encoding depends on whether the algorithm has an internal state. The internal state allows the algorithm to use the last few values inputted to help

In order to create an algorithm that

Many machine learning algorithms have no internal state. If this is the case,

establish trends.

[0.04, 0.02, -0.16]

[0.02, -0.16, 0.02]

[-0.16, 0.02, 0.04]

[0.02,0.04,0.04]

[0.04, 0.04, 0.26]

then you will typically use a sliding window algorithm to encode the data. To do this, we use the last three prices

to predict the next one. The inputs would be the last three-day prices, and the

output would be the fourth day. The above data could be organized in the following way to provide training data. These cases specified the ideal output for the given inputs.

-> 0.02

-> 0.04

-> 0.04

-> 0.26 -> -0.12

```
[0.04, 0.26, -0.12] -> -0.18

The above encoding would require
```

The above encoding would require that the algorithm have three inputs and one output.

Understanding Training

What exactly is training? Training is the process whereby an algorithm is adapted for the training data. This can be different from the "internal state" that I have mentioned. You can think of training as affecting the long-term memory of an algorithm. For a neural network, training is the weight matrix.

When training occurs depends on the algorithm. Usually, training and actual usage of the algorithm are divided into two distinct phases. Sometimes, training and usage can occur simultaneously.

Evaluating Success

In school, students are graded as they learn their subjects. There are many purposes for these grades. The most basic purpose is to provide the student with feedback on their path of learning. You must also evaluate your algorithms as they train. This evaluation will both guide the training and provide you feedback as to the success of the training.

One method of evaluation is to provide a scoring function. This scoring function takes a trained algorithm and evaluates it. The scoring function simply returns a score. The goal will be to either minimize or maximize this score. Whether any given problem is a minimization or maximization problem is purely arbitrary and is the preference of the scoring programming.

Batch and Online Training

Batch and online training usually

come into play when you are dealing with a training set, as they refer to types of learning processes. For online training, learning occurs after each training set element. Batch training accumulates learning from a certain number of elements and then the algorithm is updated accordingly. The designated number of elements is called

Online training can be useful when an algorithm must learn and train at the

the batch size. Often, the batch size is

an algorithm must learn and train at the same time. The human brain always works in this mode. However, online training is less common in AI, and not all algorithms support online training. Online training support is very common for neural networks, however.

Supervised and Unsupervised Training

This chapter outlines two different training methods: supervised and unsupervised. Supervised training

you desire from the algorithm.
Unsupervised training occurs when you do not provide the expected outputs to the algorithm.

There are also hybrid-training

occurs when you know the output that

you provide only some expected outputs. This training method is used with deep belief neural networks.

methods. In a hybrid training method,

Stochastic and Deterministic Training

A deterministic training algorithm always performs exactly the same way, given the same initial state. There are

typically no random numbers used in a deterministic training algorithm.

Stochastic training makes use of

random numbers. Because of this, an algorithm will always train differently, even with the same starting state. This can make it difficult to evaluate the effectiveness of a stochastic algorithm.

can make it difficult to evaluate the effectiveness of a stochastic algorithm. However, stochastic algorithms are very common and very effective.

Chapter Summary

This chapter provided a basic introduction to AI, particularly machine learning. You saw how problems are modeled to a machine-learning algorithm. Machine learning algorithms share some similarities to biological processes, but the goal of AI is not to exactly emulate the workings of a human brain. The goal of machine learning is to produce machines capable of some degree of intelligence beyond simple procedural programming.

Machine learning is similar to the human brain in that there is input, output, and potentially an internal state. The the output will be. This internal state can be thought of as a short-term memory that influences the output. There is also a long term memory that dictates exactly what the machine learning algorithm will

input and internal state determine what

output given the input and internal state. Training is the process of adjusting this long-term memory so that the machine learning algorithm produces the desired output.

Machine learning algorithms are typically broken into several groups: regression and classification algorithms. Regression algorithms will output a number given one or more inputs. Regression algorithms are essentially

multivariate functions. These algorithms

accept several inputs and produce an output of one or more values.

Classification algorithms accept

one or more variable to return a single class instance. They are allowed to make decisions based on the input. For example, a classification algorithm might be used to sort job applicants into preferred, average, and denied groups.

This chapter showed that the input to a machine learning algorithm is a vector of numbers. It is important to understand how to represent problems as a vector of numbers in order to pose your question to the algorithm.

The next chapter will introduce normalization. Normalization broadly

refers to the means by which data are prepared to become input for a machine learning algorithm. Additionally, normalization is used to interpret the output from the machine learning algorithm.

Chapter Normalization

- What is Normalization?
- Reciprocal Normalization and Denormalization
- Range Normalization and Denormalization

In the last chapter, we saw that a machine-learning algorithm is given a vector of floating point numbers. This is the input vector. We also saw that the machine-learning algorithm would return a vector in response to the input. This is the output vector.

present data as an input vector, as well as how to interpret the results from the output vector. In order to do so, we must learn about the several different types of data, which are all normalized in different ways.

This chapter looks at how to

Levels of Measurement

In statistics, data is typically broken down into two major categories: qualitative and quantitative. In general, quantitative data deals with quantities, or numbers. Qualitative data deals with qualities, or descriptions.

For example, consider a cup of coffee. You could describe the coffee both qualitatively and quantitatively. If you were to describe the cup of coffee qualitatively, you might list the following attributes:

Brown

- Strong aroma
- White cup
- Hot to the touch

These are all non-numerical qualities, and thus are qualitative. You can also describe the cup of coffee quantitatively.

- 12 fluid ounces
 - 106 calories
 - 65 degrees Celsius
- \$4.99 cost

These are all numeric quantities that describe the cup of coffee.

We can describe the types of data

the article "On the Theory of Scales of Measurement." (Stevens, 1946) These four data types are as follows:

• Nominal data

Ordinal dataInterval dataRatio data

in even greater detail by categorizing them into one of four subcategories. These data types were defined by psychologist Stanley Smith Stevens in

Nominal and ordinal observations are both qualitative, while interval and ratio observations are both quantitative.

The differences between each of the four can be somewhat confusing. I prefer to

mathematical operations can be used with each. This is summarized in Figure 2.1.

think of them in terms of what basic

Figure 2.1: Levels of Measurement

	Nominal	Ordinal	Interval	Ratio
* or /	No	No	No	Yes
+ or -	No	No	Yes	Yes
<0r>	No	Yes	Yes	Yes
= <u>or !</u> =	Yes	Yes	Yes	Yes
Example	Gender	Hot/warm/cold	Year	Age

of observation by considering what operators are valid on it. For example, if you have two colors, you can determine whether the two colors are equal (that is, whether both are the same color). One

You can usually determine the type

color is not greater than another color, however. You can't add two colors, nor can you multiply two colors. Given these properties, colors are nominal.

Now let's consider ordinals. The observation that something is hot or

warm indicates an implied ordering; the "hotness" of a cup of coffee is ordinal. Given two cups of coffee, one can determine whether they are the same degree of hotness and whether one is hotter than the other. Ordinals are not

clearly defined. In the case of the levels of "hotness," levels include scalding, hot, warm, room temperature, and cold.

For a slightly more complex

only ordered, but the levels of order are

example of nominal and ordinal observations, consider a zip code such as those used in the United States to allow for the quick sorting of letters and packages. They are made up of six digits, and each specifies a particular region. For example, the 90210 zip code

specifies an address in Beverly Hills,

California.

Although zip codes are always made up of digits and look like numbers, they are not numbers. You could compare two zip codes to see if they are

answer. So a zip code is clearly qualitative, rather than quantitative. But is it nominal or ordinal? Although one could compare the numerical value of zip codes to say that one zip code is greater than another, the higher value of a zip code gives it no special meaning. Certainly, higher zip codes are often in the west of the USA and lower zip codes often specify a location in the east, but this tendency does not hold true in all cases. Zip codes, therefore, are nominal.

equal, but to add to or subtract from a zip code would give a meaningless

Quantitative Observations

Now we will look at quantitative

nominal. In addition to the operators above, I will give you one additional rule to define the difference. Interval observations have an arbitrary zero, whereas ratio observations have an actual non-arbitrary zero that defines their beginning. For example, age is a ratio. It has a clearly defined origin at zero, for there are no ages before age 0. The current

observations. The relationship between interval and ratio can be a little more complex than between ordinal and

0. Let's apply the operator test to

year, on the other hand, is an interval. It does not have a clearly defined origin at

else, so the multiplier rule is a yes, which defines age as a ratio. You could treat the current year as a number and multiply it by 2, but that would not mean that one date was twice the other, because dates do not have an origin at 0. However, you may add and subtract quantities from dates to get meaning, so the current date does count as an interval. Temperature can be either a ratio

these two examples. You can say that someone is twice the age of someone

or an interval, depending on the scale used. If you measure the temperature in Kelvin, then zero is absolute zero; thus, temperature measured in Kelvin is a ratio. Temperature measured in

Fahrenheit or Celsius is an interval, on the other hand, because zero is not the origin for either Fahrenheit or Celsius. Test this definition using the phrase

"twice as hot." Ten degrees Celsius cannot be twice as hot as five degrees Celsius, for there are an infinite number

of degrees available below 0. Thus, because the term "twice" has no meaning with Celsius or Fahrenheit, they are intervals rather than ratios.

With Kelvin, zero is absolute zero—there is no molecular movement at all, and it cannot possibly be colder than 0. In the case of Kelvin, 0 is the true origin

point. Twice as hot as 5 is in fact 10

degrees, in Kelvin.

kilometers per hour. There is no going slower than zero kilometers per hour, and so zero is the true origin point.

as fast as five kilometers per hour is ten

Similarly, speeds are ratios: twice

Most scientific measurements are ratio observations. These include length, width, electrical charge, volume, mass, and Kelvin temperature. The value of interval measurements are still helpful trackers, but typically their meaning is more arbitrary.

Normalizing Observations

In the previous chapter we saw that all input and output from machine learning algorithms are typically vectors of floating point numbers. The real world observations that we provide to a machine learning algorithm must be nominal, ordinal, interval, or ratio. Nominal and ordinal observations are not inherently numeric, so we need to convert these into a number that is meaningful to the machine learning algorithm.

Some machine learning algorithms require that all observations be in a specific range, usually -1 to +1 or 0 to

+1. Even if you are not required to be in a specific range, it is often a good idea to ensure that your values fall into a range. This will normalize the values so they can be compared.

Why is normalization necessary?

Consider if you made two observations, one of which was the daily volume of the NYSE and the other of which was the point movement of an individual stock. The NYSE daily volume is usually in the billions, while the number of points moved by many individual stocks is typically less than 10. The volume number could easily overwhelm the point movement, making the point movement seem meaningless, or zero.

Normalization is something we see

forms is that of percentages. If something is 5% off, you can easily tell the relative size of the discount. It might be a few dollars for a new cell phone or it might be several hundred dollars for a car, yet the size of the percentage figure stays the

same. We could normalize the values in the NYSE example by considering them as percentages. Now we might say that

every day. One of its most common

the volume increased by 10%, while the stock fell by 5%. The volume number is now comparable to the point number.

In the next sections we will see how to normalize nominal, ordinal,

Normalizing Nominal

interval, and ratio observations.

Observations

There are two commonly used methods for normalizing ordinal values. In this section, we will look at one-of-n encoding. This the most simple means of normalizing nominal values. Later in this chapter, we will discuss equilateral encoding. Equilateral encoding is more complex, but is often more efficient than one-of-n encoding.

One-of-n is a very simple form of normalization. For an example, consider the iris dataset that we saw in the last chapter. A single line from the iris data set is shown here. The species is non-numeric. We will have to use one-of-n

normalization for it.

5.1,3.5,1.4,0.2,Iris-setosa

The first four values are all ratio observations, as they are lengths and the origin is at zero. However, the fifth value is nominal, which is sometimes called categorical. It describes a category. The nominal value is defined by the species of the iris; in the iris dataset described above, there were three iris species:

- Setosa
- Versicolor
- Virginica

the machine learning algorithm would have three outputs—one for each iris species. The machine learning algorithm would most likely be trained to accept the four length measurements as inputs and then output three values to predict what species of iris the input data corresponds to.

With the one-of-n normalization,

Normalization is used to create training data. A machine learning algorithm is trained with training data. The actual process of training will be covered later in this book. For now, you simply need to be aware that a training set is a collection of input vectors that includes the ideal output for each vector. We can use the iris data set to generate a

training set. First, to generate the inputs, we will normalize each of the four ratio observations. Later in the chapter we will see how to normalize ratio observations. For now, we will focus on the species.

Generating the ideal output for each of these input vectors is relatively easy. Simply assign a +1 to the neuron that corresponds to the chosen iris and a -1 to the remaining neurons. For example, using a normalization range of -1 to 1, the Setosa iris species would be encoded as follows:

1,-1,-1

Likewise, the Versicolor would be

Finally, Virginica would be encoded as follows.

encoded as follows:

-1,1,-1

If you are using 0 to 1, then substitute 0 for the -1 values in the above three species encodings.

Normalizing Ordinal Observations

Ordinal observations are not necessarily numeric. However, they do have an implied ordering. For example,

progressed through by a student in the United States. One moves from preschool level to senior level before graduating. The levels have no true numerical value, but they do occur in a set order.

In order to normalize an ordinal set,

consider the levels of education

one must preserve the order. One-of-n encoding loses the order. While the outputs are a vector, and it may appear that there is order, there is really no ordering, because most machine learning algorithms treat the individual outputs with no ordering at all. Just because output #1 and output #2 are next to each other, that does not mean they are in any

way related. Implying such ordering might introduce bias.

To normalize ordinal observations,

there two options. First, you can simply normalize with one-of-n encoding and forget the order. It could be that the order is not important, and in that case you can simply treat the observation as unordered nominal data set. However, if you wish to preserve the order, you need to assign a whole number to each category, starting with zero. The number assignments for the grades would thus be as follows:

- Preschool (0)
- Kindergarten (1)

- First grade (2)
 Second grade (3)
 Third grade (4)
- Third grade (4)Fourth grade (5)
- Fifth grade (6)
- Sixth grade (7)
- Seventh grade (8)Eighth grade (9)
- Freshman (10)
- Sophomore (11)Junior (12)
- Senior (13)

Now, we calculate a percent completion rate to determine the value for each level. There are fourteen total categories. So someone in sixth grade has completed 50% of their education.

range 0 to 1, then the percentage is sufficient at 0.5. However, if we are

If we are normalizing between the

7 / 14 = 0.5 (50%)

1)) = 2

normalizing to the range -1 to 1, we need to apply the percent to that range. In order to do so, calculate the width of the range, which is the high value of the range subtracted by the low value.

width = (high - low) = (1 - (-

The percentage can be applied to the value of the width. If we are 50%,

the value of the width. If we are 50%, then we are halfway. Simply multiply the percent by the width.

widthDistance = width * 0.5 = 1

Now, add the width to the lower bound to get the normalized number. If we had achieved zero percent, we would be exactly at the lower bound (-1). If we had achieved one hundred percent, we would be exactly at the upper bound (+1). Sixth grade thus normalizes to 0.

lowerBound + widthDistance =
$$-1 + 1 = 0$$

The above process can be summarized using Equation 2.1:

Equation 2.1: Normalize Ordinal Observation

$$f(x) = \frac{(n_H - n_L)x}{N} + n_L$$

normalize the percentage is one that will be used again and again. The next two normalization techniques will build on that concept. For example, the next section shows how to reverse this process and denormalize a normalized ordinal observation. **Ordinal Denormalizing Observations** Denormalization is the opposite of

normalization—it allows you to take a number that was normalized and convert it back to the original number. This is

The concept of calculating the

width between the high and low values and taking the percent of that width to predict the grade level achievement of any given person, based on other observations, you would probably train the algorithm with current grade level observations that were normalized. Because the algorithm was trained with normalized data, it will also output normalized data. You need to denormalize this output so that it will have meaning in the context of the knowledge that you hoped to achieve. I will now show you how to denormalize the grade level from the

previous section, which is essentially

very useful when processing the output from a machine learning algorithm. For example, if you trained an algorithm to steps in reverse. Let's say that the output is the normalized value of zero. To determine what grade that represents, we first need to calculate how far it is from the lower bound:

the process of running the normalization

widthDistance = 0 - (-1) = 1

normalized.

This converts our distance into the width. We can determine the percentage by calculating what percent into the width the above distance describes. We know the total width, because it is the range between the normalized upper and lower bounds (-1 and 1). In order to denormalize, you must know the range in which the data were originally

We now apply this 50% to our total number of categories, which, in this

widthPercent = widthDistance / w:

categoryNumber = totalCategories

case, is 14.

The list giving value to the grades indicates that 7 corresponds to the sixth grade. We have thus denormalized the observation.

The above process can be summarized using Equation 2.2.

Equation 2.2: Denormalize Ordinal Observation

$$f(x) = \frac{N \cdot (x - n_L)}{n_H - n_L}$$

In the next section, we will see how to normalize quantitative observations.

Normalizing Quantitative Observations

Interval and ratio observations are normalized in the same way. We simply look at the range from which either of the quantitative observation types are drawn and normalize them to the desired range. The individual qualities that make an interval observation different from a ratio observation are meaningless for normalization.

Quantitative observations are always numeric, so they might not need

learning algorithms do require that numeric data be normalized to a specific range, some do not. It is important to know the numeric ranges required by the algorithm you are using in order to receive relevant output.

to be normalized. While many machine-

For practice, let's normalize the weight of an automobile. For the purposes of this example, I will estimate that the range for the weight of a car is between 100 and 4,000 kilograms. As mentioned in Chapter 1, the guessed low should be lower than the real low and the guessed high should be higher than

the actual high. I would like to normalize this range between -1 and 1. The various highs and lows that apply to this dataHigh: The highest unnormalized

scenario are listed as follows:

observation

- dataLow: The lowest unnormalized observation.
- normalizedHigh: The high end of the range to which the data will be normalized.
- normalizedLow: The low end of the range to which the data will be normalized.

Plugging in the values from above provides the following values:

• dataHigh: 4,000

- dataLow: 100
- normalizedHigh: 1
- normalizedLow: -1

We can now normalize the data. We need to calculate two ranges, or widths: dataHigh to dataLow and normalizedHigh to normalizedLow.

```
dataRange = dataHigh - dataLow =
normalizedRange = normalizedHigh
1) = 2
```

Let's attempt to normalize a car weight of 1,000 kilograms. First, we need to determine how far into the dataRange this value is.

d = sample - dataLow = 1000 - 100

We now convert this to a percent.

dPct = d / dataRange = 900 / 3900

Rounded, this gives 0.23. We now calculate how far into the **normalizedRange** is 0.23.

dNorm = dRange * dPct = 2 * 0.23

We now add this to the normalized low, and we are done.

Normalized = normalizedLow + dNo: 1 + 0.46 = -0.54

The normalized value is -0.54.

The above process can be summarized using Equation 2.3.

Equation 2.3: Normalize Quantitative Observation

$$f(x) = \frac{(x-d_L)(n_H-n_L)}{(d_H-d_L)} + n_L$$

The next section will show how to reverse this process and denormalize a quantitative observation.

Denormalizing Quantitative Observations

To denormalize a quantitative observation, the normalization process is reversed. Let's use the normalized - 0.54 from before. First, we calculate how far it is from the lower bound.

-0.54 - (-1) = 0.46

by the distance between the normalized min and max. 0.46 / 2 = 0.23

We now need to divide this number

The result is 0.23, or 23%. Multiply this by **dataRange**.

0.23 * 3900 = 897

The value 897 is the distance into the **dataRange** that we are. To convert this to an actual weight, just add **dataLow**.

897 + dataLow = 897 + 100 = 997

The value 997 is approximately equal to our original number of 1,000, so

we have denormalized the weight. It is not exactly equal because I rounded on some of the divisions.

The above process can be summarized with Equation 2.4.

Equation 2.4: Denormalize Quantitative Observation

$$f(x) = \frac{(d_L - d_H)x - (n_H \cdot d_L) + d_H \cdot n_L}{(n_L - n_H)}$$

There are other ways to normalize both nominal and quantitative observations. These will be covered in the next section.

Normalization There are many other means of normalizing observations. The means

Other Methods

already presented are the most common. This section will introduce some other normalization methods for both quantitative and nominal observations.

Reciprocal Normalization

In this section we will look at a very simple means of normalization—reciprocal normalization. This normalization method supports both

normalization and denormalization. However, reciprocal normalization is the range of your choice. Rather, reciprocal normalization always normalizes to a number in the range between -1 and 1.

Reciprocal normalization is very

limited in that you cannot normalize into

easy to implement. It requires no analysis of the data to determine high and low data values. Equation 2.5 shows how to use reciprocal normalization.

Equation 2.5: Reciprocal Normalization

$$f(x) = \frac{1}{x}$$

To see Equation 2.5 in use, consider normalizing the number five.

As you can see the number five has

f(5.0) = 1.0/5.0 = 0.2

As you can see, the number five has been normalized to 0.2.

Reciprocal Denormalization

It is very easy to denormalize a number that has been normalized reciprocally. Because it is a reciprocal, it is the same equation.

Equation 2.6: Reciprocal Denormalization

$$f(x) = \frac{1}{x}$$

To see Equation 2.6 in use, consider denormalizing the number 0.2.

f(0.2) = 1/(0.2) = 5.0

As you can see, we have easily completed a round trip. We normalized 5.0 to 0.2, and then denormalized 0.2 back to 5.0.

Understanding Equilateral Encoding

Equilateral encoding is a potential replacement for one-of-n encoding. I must admit that I am rather fond of this encoding method. If you've read my web-based articles, you will see that I use it often. Equilateral encoding brings two main features to the table.

• Requires one fewer output than

- one-of-nSpreads the "blame" better than one-of-n
- Equilateral encoding uses one fewer output than one-of-n. This means that if you have ten categories to encode, one-of-n will require ten outputs while equilateral will require only nine. This gives you a slight performance boost.

The second feature is slightly more difficult to understand. Most training algorithms will score the output of a machine-learning algorithm based on the incorrectness of each output. Consider if you had 100 categories, which would require 100 outputs in one-of-n. The incorrectness will be centered primarily

output would be as follows:

output. All of the other outputs have an "ideal value" of either 0 or -1, depending on your normalization range. This can cause a small problem for the one-of-n normalization method. If the algorithm had predicted a versicolor iris when it should have predicted a verginica iris, the actual output and ideal

on two outputs. Recall that one-of-n specifies the selected category by which output has the highest value. The two outputs primarily involved in the incorrect answer are the output that mistakenly had the highest output and the output that should have had the correct

Ideal output: -1, -1, 1

The problem is that only two of three actual outputs are incorrect. We would like to spread the "guilt" for this error over a larger percent of the actual outputs. This ensures that any training correct is applied equally to all outputs. To do this, a unique set of values for each class must be determined. Each set of values should have an equal Euclidean distance from the others. We will see more about Euclidean distance later in this chapter. The equal distance makes sure that incorrectly choosing Iris setosa for versicolor has the same error weight as choosing Iris setosa for Iris virginica.

Listing 2.1 shows the ideal classes normalized for one of n.

Listing 2.1: Calculated Class Equilateral Values 3 Classes

```
0: -0.8660 , -0.5000
1: -0.8660 , -0.5000
2: 0.0000 , 1.0000
```

for each of the three classes. This causes the decreased number of outputs provided by equilateral encoding relative to one-of-n encoding. Equilateral encoding always requires one fewer output than one-of-n encoding would have.

Notice that there are two outputs

equilateral normalization. Just as before, consider whether the algorithm had predicted a versicolor iris when it should have predicted a verginica iris. The output and ideal are as follows:

Look at the example concerning

Ideal output: 0.0000 , -1.0000 Actual output: -0.8660 , -0.5000

In this case, there are only two

outputs, as is consistent with equilateral encoding. Now all outputs are producing incorrect values. Additionally, there are only two outputs to process, which slightly decreases the amount of data processed by the machine learning algorithm.

Algorithms will rarely give output

work for equilateral encoding. Equilateral encoding shows what calculated class equilateral value (Listing 2.1) has the shortest distance to the actual output of the algorithm.

that exactly matches any of their training values. To deal with this in one-of-n encoding, we simply look at what output was the highest. This method does not

What is meant by the assertion that each of the sets are equal in distance from each other? It means that their Euclidean distance is equal. Distances will be covered in greater detail in the next chapter. The Euclidean distance can be calculated using Equation 2.7.

Equation 2.7: Euclidean Distance

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

In the above equation, the variable

"q" represents the ideal output value; the variable "p" represents the actual output value. There are "n" sets of ideal and actual outputs. The next chapter will greatly expand upon Euclidean distance.

Implementing Equilateral Encoding

I will now show you the means by which the Euclidean encodings are calculated. I originally saw this algorithm in the book "Practical Neural

Network Recipes in C++" by Masters (1993), who cited an article in PCAI as the actual source. (Guiver, 1991)

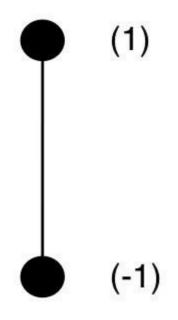
The equilateral algorithm can be a bit confusing, so I will demonstrate it in two different ways. First, I will demonstrate it graphically. We will

normalize to the range -1 to 1. Consider if we were to simply encode two

categories. Equilateral encoding requires one output less than the number of categories. For two categories, only one output is given. We can think of the single output as a single dimension. Figure 2.2 demonstrates what the one-

Figure 2.2: Equilateral Encoding for Two Categories

dimensional output will look like.



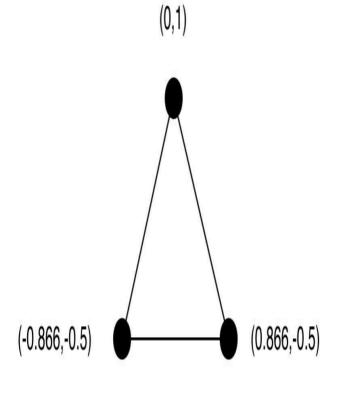
You can see the two points on the above line. We would have a single output of either 1 or -1.

two dimensions; it creates an equilateral triangle. This is where the name equilateral encoding comes from. Figure 2.3 shows how the three categories are encoded.

would be two outputs. Think of this as

If we had three categories, there

Figure 2.3: Equilateral Encoding for Three Categories



categories must be equally distant from their neighbors. This allows the three categories to be represented in two dimensions. The dimensions that you see in the above figure match the encodings that we used in Figure 2.2.

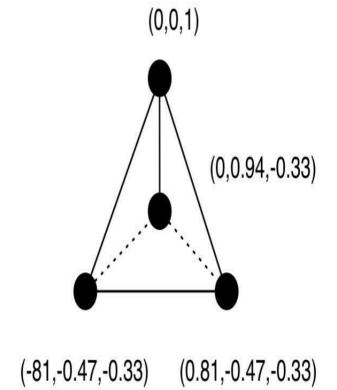
encoding is that each of these three

The key point of equilateral

categories. To encode four categories, we need three outputs, or three dimensions. This is depicted in in Figure 2.4.

We can also encode four

Figure 2.4: Equilateral Encoding for Four Categories



essentially a triangle-based pyramid. Just like all equilateral triangles, the lengths of all sides are equal.

dimensional equilateral triangle. It is

The above figure is a three-

We can also encode much larger

numbers of categories. I cannot show these as dimensions because it is difficult to display a high dimensional figure in our three dimensional world, let alone on a two-dimensional book page.

let alone on a two-dimensional book page.

Hopefully the graphical representations above show how the categories are arranged equidistantly from one another. Now I will show you how these numbers are actually

calculated.

matrix. The matrix is **N** by **N**-1, where **N** is the number of categories. Each row contains the encodings for one category. We will always create this matrix for normalization to the range -1 to 1. We will ultimately scale the completed matrix to whatever range we desire.

is usually implemented to output a

The equilateral encoding algorithm

To begin creating this matrix we first seed the matrix for a two class encoding. As seen in Figure 2.1, this is simply the values -1 and 1. We begin by seeding these two values into the matrix.

```
result[0][0] = -1;
result[1][0] = 1;
```

We will now loop from two

categories up to our N classes. We skip 1 because we already seeded for the case where we have one category only. We loop from 2 up to, but not including, N.

```
for k from 2 to N {
```

Next, we calculate a scaling factor. We will recursively build each successive matrix from the previous matrix. We seed for two categories, and then scale it to build the matrix for three categories. This is done with the following code:

```
f = sqrt(N * N - 1.0) / r;
```

Next, we loop over the portion of

calculated and scale.

for i from 0 to k {

the matrix that we have already

```
for j from 0 to k-1 {
    result[i][j] *= f;
}
```

We will now populate the edge of the matrix (columns) with the negative reciprocal of N.

```
r = -1 / N;
for i from 0 to k {
   result[i][k - 1] = r;
}
```

Set the last value in the matrix to 1.0 and continue the previous "for loop."

```
result[k][k - 1] = 1.0;
}
```

Now that the loop is complete, we are ready to scale the matrix to the appropriate range. We use the same normalization formula shown in Equation 2.3.

We will use -1 and 1 for the low and high ranges for the data.

```
dataLow = -1;

dataHigh = 1;
```

for row from 0 to N {

We now loop over the entire matrix and scale it.

```
for col from 0 to N-1 {
          result[row]
```

[col]

((result[row]

ready to be used as a table for equilateral encoding. If you wish to encode a category to equilateral, simply use the matrix as a lookup table and copy the row that corresponds to the category you are encoding. To decode, simply find the matrix row that has the lowest Euclidean distance to the output vector from your machine-learning algorithm.

Chapter Summary

This chapter described several normalization processes. Normalization is the process by which data is forced to conform to a specific range. The range is usually either -1 to +1 or 0 to 1. The range you choose is usually dependent on the machine-learning algorithm you are using. This chapter covered several different types of normalization.

Reciprocal normalization is a very simple normalization technique. This technique normalizes numbers to the range -1 to 1. Reciprocal normalization simply takes the reciprocal normalization and divides the number to

Range normalization is more complex. However, range normalization

normalize by 1.

allows you to normalize to any range you like. Additionally, range normalization must know the range of the input data. While this does allow you to make use of the entire normalization range, it also

means that the entire data set must be

analyzed ahead of time.

This chapter also showed how Euclidean distance can be used to determine how similar two vectors are to one another. The next chapter will expand upon the concept of distance and

introduce additional distance metrics.

Chapter 3: Distance Metrics

- Vectors
- Euclidean Distance
- Manhattan Distance
- Chebyshev Distance

Distance is a very important measurement in both real life and Artificial Intelligence (AI). In real life, distance measures the degree of separation between two points. In AI, distance is used to calculate the similarity of two vectors. For AI, think of a vector as a one-dimensional array—



Understanding Vectors

A vector is essentially a onedimension array. Do not confuse the dimensionality of the vector array with the dimensions of your problem. Even if your problem had 10 inputs, you would still have a vector. Vectors are always one dimension arrays. Your ten inputs would be stored in a vector of length ten.

In AI, a vector is usually used to store observations about a particular instance of something.

This maps to the real world concept of distance quite well. You can think of a point on a sheet of paper as having two dimensions, which are

a point in 3D space has three dimensions, usually labeled "x," "y," and "z." A two dimensional point can be stored in a vector of length two. Likewise, a 3D point can be stored in a

usually referred to as x and y. Likewise,

Our universe is made up of three perceivable dimensions, although sometimes "time" is treated as a fourth dimension. However, this is a manifold, and does not imply that time is a true dimension at least in the sense of the

and does not imply that time is a true dimension, at least in the sense of the first three. Because higher dimensions are imperceptible to humans, it is very difficult for us to comprehend dimensional spaces higher than three. Very high dimension spaces are very

common in AI, however.

Recall from Chapter 2,
"Normalizing Data" that the iris data set

"Normalizing Data," that the iris data set had the following five observations, or features:

- Sepal length
 - Sepal width
 - Petal length
 - Petal width
 - Iris species

You could think of this data set as a vector of length 5. However, the species feature must be handled differently than the other four. Vectors typically contain only numbers. The first four features are

inherently numerical, but species is not. As demonstrated in chapter two, there are several ways to encode the species observation to additional dimensions.

Only simple numeric encoding

translates the iris species to a single

dimension. We must use additional dimensional encodings, such as one-of-n or equilateral, so that the species encodings are equidistant from each other. If we are classifying irises, we do not want our means of encoding to

other. If we are classifying irises, we do not want our means of encoding to induce any biases.

Thinking of the iris features as dimensions in a higher dimensional space makes a great deal of sense. You

can think of the individual samples (the rows in the iris data set) as points in this

search space. Points closer together are likely to share similarities. Let's take a look at what this actually looks like by considering the following three rows from the iris data set:

5.1, 3.5, 1.4, 0.2, Iris-setosa

If we use one-of-n encoding to the range 0 to 1, the above three rows would encode to the following three vectors:

7.0,3.2,4.7,1.4, Iris-versicolor 6.3,3.3,6.0,2.5, Iris-virginica

[5.1,3.5,1.4,0.2,1,0,0] [7.0,3.2,4.7,1.4,0,1,0] [6.3,3.3,6.0,2.5,0,0,1]

Now that you have the data in vector form, you can calculate the

distance between any two data items. The next few sections will describe several different methods to calculate the distance between two vectors.

Calculating Vector Distance

The distance between two vectors tells us the degree of similarity between two vectors. There are several different ways to calculate this vector distance.

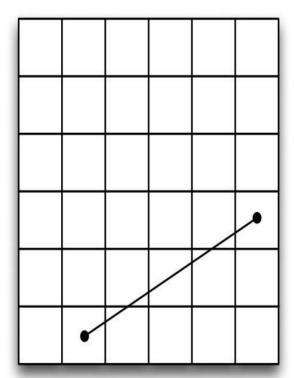
Euclidean Distance

The Euclidean distance measurement is based off of the real, two-dimensional distance between two vectors. That is, it is the difference between the two points if you drew them on paper and measured with a ruler. This two-dimensional distance is based on the Pythagorean Theorem. Specifically, if you had two points

between the two would be described as follows: $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

(x1,y1) and (x2,y2), the distance

Figure 3.1: Two-Dimensional Euclidean Distance



comparing two vectors of length two. However, most vectors are longer than two numbers. To calculate the Euclidean distance for any sized vector, use the general form of the Euclidean distance equation.

This would work fine for

The Euclidean distance measurement is used often in Machine Learning. It is a quick way to compare two vectors of numbers that have the same number of elements. Consider three vectors, named vector **a**, vector **b**, and vector **a**. The Euclidean distance

and vector **c**. The Euclidean distance between array **a** and array **b** is 10. The Euclidean distance between array **a** and array **c** is 20. In this case, the contents of array **a** more closely match array **b** than

they do array **c**.

Equation 3.1 shows the formula for calculating the Euclidean distance

calculating the Euclidean distance. (Deza, 2009)

Equation 3.1: The Euclidean Distance

$$d(\mathbf{p}, \mathbf{q}) = d(\mathbf{q}, \mathbf{p}) = \sqrt{\sum_{i=1}^{n} (q_i - p_i)^2}$$

The above equation shows us the

Euclidean distance \mathbf{d} between two arrays \mathbf{p} and \mathbf{q} . The above equation also states that $\mathbf{d}(\mathbf{p},\mathbf{q})$ is the same as $\mathbf{d}(\mathbf{q},\mathbf{p})$. This simply means that the distance is the same no matter which end you start at. Calculation of the Euclidean distance is no more than summing the squares of

Following this, the square root of this sum is taken. This square root is the Euclidean distance.

The following shows Equation 3.1

the difference of each array element.

The following shows Equation 3.1 in pseudo code form.

function euclidean (position1, po

```
{
  sum = 0;
  for i from 0 to position1.lengt
  {
    d = position1[i] - position2
    sum = sum + d * d;
  }
  return sqrt(sum);
```

Manhattan Distance

}

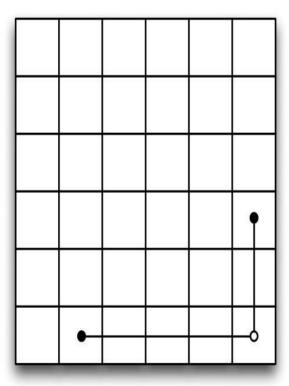
Euclidean distance can be thought of in terms of "as the crow flies." Manhattan distance calculates the distance as

commonly called taxicab distance.

Manhattan distance is also

though you were driving on a city grid. (Krause, 2012) You can see two-dimensional Manhattan distance depicted in Figure 3.2.

Figure 3.2: Two-Dimension Manhattan Distance



To calculate the Manhattan Distance between two points, add the absolute distances of each of the dimensions. Equation 3.2 performs this operation. (Deza, 2009)

Equation 3.2: The Manhattan Distance

$$d(\mathbf{p}, \mathbf{q}) = d(\mathbf{q}, \mathbf{p}) = \sum_{i=1} |p_i - q_i|$$

The primary difference between the Euclidean and Manhattan distances is that large distances are penalized disproportionately more than small distances. For example, when using Euclidean distance, the distance between two vectors that differ by one unit in two

vectors that differ by two units in only one dimension (two), whereas they would both be equal (two) using Manhattan distance.

in pseudo code form.

return sum;

The following shows Equation 3.2

dimensions (the square root of two) is less than the distance between two

```
function manhattan (position1, po
{
   sum = 0;
   for i from 0 to position1.lengt
   {
      d = abs(position1[i] - posit:
      sum = sum + d;
   }
}
```

Chebyshev Distance

The Chebyshev distance is also commonly called the chessboard distance. If you've ever played chess, you can think of it as the number of moves that a king would take to move between the two points. Figure 3.3 shows how far each of the locations is from the first point.

Figure 3.3: Two-Dimension Chebyshev Distance

4	4	4	4	4	4
3	3	3	3	3	3
2	2	2	2	2	3
2	1	1	1	2	3
2	1	•	1	2	3
2	1	1	1	2	3

distances, take the maximum of the dimension differences. This is described in Equation 3.3. (Deza, 2009)

Equation 3.3: The Chebyshev

To calculate the Chebyshev

Distance

$$d(\mathbf{p}, \mathbf{q}) = d(\mathbf{q}, \mathbf{p}) = \max_{i} (|p_i - q_i|)$$

The Chebyshev distance can be useful when you want to focus on the dimension with the largest distance. When all dimensions are either normalized or in approximately the same range and the worst dimension governs the similarity between the two vectors, the Chebyshev distance is best to use.

The following shows Equation 3.3

```
in pseudo code form.
function chebyshev (position1, po
{
  result = 0;
  for i from 0 to position1.lengt
    d = abs(position1[i] - posit:
    result = max(result, d);
  }
  return result;
}
```

Optical Recognition

Character on

OCR is a very common example of machine learning. You've probably seen it on the Internet. Most of these examples are of the same form. You draw a series of characters and a very complex machine-learning algorithm (often a neural network) learns your characters and can recognize new ones.

Euclidean distance can be used to perform basic Optical Character Recognition (OCR). The program allows you to draw individual characters and add them a list of known characters. The characters you draw are

input for AI. This section describes how to normalize an image using down sampling. There are more advanced methods than this, but down sampling is often effective. (Lyons, 2009)

images, which are a popular source of

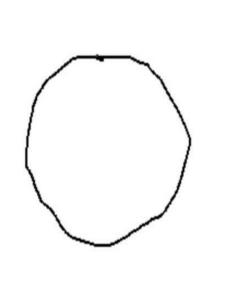
often effective. (Lyons, 2009)

The first step is to take a raw image that you want the program to recognize. A real OCR package would have to process the image and determine its individual characters. For this example, we will simplify the process by only

using a single character. Figure 3.4

shows such an image—a zero digit.

Figure 3.4: Drawing a Zero



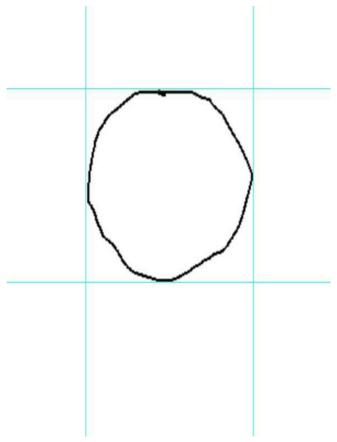
a bit of extra space at the sides of the digit I drew. This could present a problem. The machine learning algorithm will be looking at a grid of pixels as inputs. What if the user draws the zero in the upper left corner during training, but in the lower-right corner when actually using the algorithm? The algorithm would be unlikely to recognize the second drawing, because the pixels would be on different inputs. Because of this, it is necessary to crop. To crop, just

drop lines from the top, left, right, and bottom until they touch a pixel. Figure

You may have noticed there is quite

Figure 3.5: Cropping the Digit

3.5 shows the cropping lines.



so, we will also down sample. This will cause us to have fewer pixels to review and resolves issues related to size. If the user draws the digit at different sizes, down sampling will eliminate the possibility that the sizing will affect the program's reading.

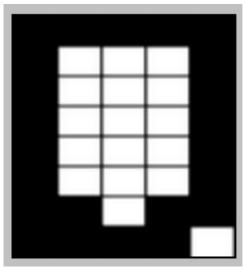
Then crop the image. While doing

Why do we need to decrease the number of pixels? Consider a full-color image that is 300x300 pixels. We would have 90,000 pixels times the three RGB colors, giving 270,000 total pixels. If we had an input for each pixel, that would be 270,000 inputs. Each image is a vector, and a 270k-dimension vector would be very large! To make the program more robust, it is necessary to decrease the number of inputs.

Figure 3.6 shows what the image

Figure 3.6 shows what the image looks like down sampled to 7x5 pixels.

Figure 3.6: Down Sampling



7x5 grid over the high-resolution image. For each grid cell, make the entire cell black, if even one underlying pixel is black.

To perform the down sample, lay a

Because we have a 7x5 grid, we

now can create a vector of size 7x5 or 35 inputs. We create a vector for each digit and store its cropped, down sampled form in a table. When the user draws new characters to recognize, we will crop and down sample. A new vector is created for each image. We then find the digit in our table with the least distance from our new image. We determine the new image to be the same digit as the digit in the table with the lowest distance.

Chapter Summary

Vectors are a very important component of machine learning. Both input and output are in the form of vectors in the context of a machine learning algorithm. The memory of the machine learning algorithm is typically thought of as a vector. Vectors can also be considered as coordinates in an ndimensional space. This allows us to compare the similarity of two vectors by computing the distance between them.

There are many different ways to calculate the distance between two vectors. One of the most basic is Euclidean distance. Euclidean distance

between two-dimensional points. This same formula can be applied to any number of dimensions. Manhattan distance and Chebyshev distance may also be used.

uses the regular distance formula for

Optical Character Recognition (OCR) can be implemented through simple distance calculation. We begin by creating a table of known characters and a table of vectors to represent these characters. These vectors are created by cropping and down sampling the character images. New images are cropped and down sampled, as well. We then determine the new character to be the character that has the least distance from one of the vectors stored in the Random numbers are a very important concept to machine learning.

table.

We will often use a random vector as the initial state of a machine learning algorithm. This initial random state is then refined during training. Random numbers can also be used for Monte Carlo techniques for training. The next chapter will cover random numbers.

Chapter 4: Random Number Generation

- Pseudorandom Number Generation
- Linear Congruential Generator (LCG)
 Multiply With Carry (MWC)
- Mersenne Twister
- Monte Carlo Method

Random numbers are very important to many machine learning algorithms and training techniques. When performed by computers, random

When performed by computers, random number generation is called pseudorandom number generation that something is implied, rather than defined. This is the case with computer generated random numbers, as a computer is a completely logical machine that follows instructions and can only simulate randomization. Given

(PRNG). The prefix "pseudo" means

exactly the same inputs and internal state, a computer will always produce exactly the same outputs. (Turing, 1948)

Despite these logical limitations to randomization, computers can be very

randomization, computers can be very effective at pseudorandom number generation. Two criteria are often used to judge the effectiveness of a PRNG: the randomness of the algorithm and the security of the PRNG algorithm. An algorithm can be very random, but is not

randomness of an algorithm. Security is more important for an encryption algorithm. A secure PRNG is called a Cryptographically Secure Pseudorandom Number Generator (CSPRNG).

Good randomness is defined by whether a PRNG's period produces

necessarily cryptographically secure. For AI, we care primarily about the

detectable repeating sequences within a period and how long the PRNG's periods are. In this context, a period is the amount of random numbers that a PRNG can produce before it begins to repeat the sequence. Each period is essentially a string of numbers, and each PRNG compiles a series of identical periods. The larger the period, the more random a generator is. The fewer repeating sequences evident inside of a period there are, the more random a generator is.

It is important to understand the

distinction between regular PRNGs and CSPRNGs. All PRNGs and CSPRNGs have an internal state. If you know the internal state of the generator, you will know what the next random number will be. PRNGs and CSPRNGs can both potentially produce high quality random

potentially produce high quality random number sequences. The primary difference between PRNGs and CSPRNGs is that you can typically determine a PRNG's internal state by analyzing the numbers. However, you cannot determine a CSPRNG's internal This distinction is critical for cryptology, but is not as important for AI. In AI, the quality of the numbers is most important, while the numbers' likelihood of providing information about the algorithm's internal state is of

less importance.

state in a reasonable amount of time.

PRNG Concepts

There are several important concepts that nearly all PRNGs share. These define how the PRNG performs and what its expected output can be. Common concepts that all PRNGs share include the following:

- Seed
- Internal State
- Period

The seed defines the sequence of random numbers you will get, as well as the initial internal state. You should always get the same sequence of random nearly every seed should produce a different sequence of random numbers.

The internal state comprises the

variables that the PRGN uses to produce

numbers for the same given seed, and

both the random numbers and the next internal state. If you know the internal state and the type of PRGN or CSPRNG algorithm, you can predict the next random number.

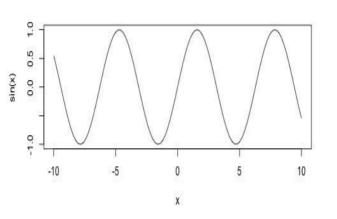
The length of each random number sequence is the period. Once the period is up, the random PRGN will repeat. That is why the PRGN is considered a

That is why the PRGN is considered a periodic function—because it repeats its values at regular intervals or periods. Figure 4.1 shows the sine function,

which is perhaps the most well-known

periodic function.

Figure 4.1: The Sine Function is Periodic



As you can see from the above figure, the sine function has a period of

2*PI, or approximately 6.18.

Random Distribution Types

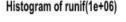
You will usually want your random

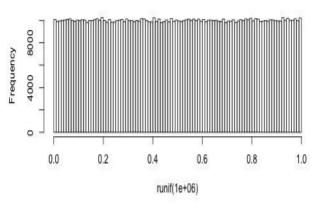
numbers to be uniformly distributed. PRNGs typically provide a random number between 0 and 1, with equal probability of getting any particular number in that range. You can see the results of generating a large number of random numbers between 0 and 1 in

Figure 4.2, which shows a uniform

Figure 4.2: Uniform Distribution of Random Numbers

distribution of random numbers.





As you can see from figure 4.2 above, the random numbers are evenly distributed between 0 and 1. This is called a uniform distribution, or a uniform random number. It provides equal probability of getting any option

within the specified range.

Most programming languages

provide a means to generate uniformly

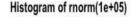
provide a means to generate uniformly distributed random numbers between 0 and 1. You can scale this random number out to whatever range you desire. This works very similarly to normalization. If the function **rand()** returns a random number between 0 and 1, then equation 4.1 scales it to a range between **high** and **low**.

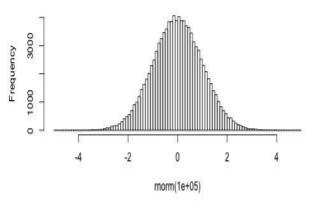
Equation 4.1: Random Numbers in a Range

 $rnd(low, high) = rnd() \cdot (high - low) + low$ The above equation allows you to generate a random number in any range. provide a means to generate a normally distributed random number. Figure 4.3 shows such normally distributed random numbers.

Some programming languages also

Figure 4.3: Normal Distribution of Random Numbers





The random numbers with the greatest probability are clustered around 0. There is really no defined upper and lower bound. Each whole number represents a standard deviation. As the standard deviations increase on both the

probability of getting a random number decreases greatly. Beyond 4 or -4, it is very rare to get a number. Normally distributed random numbers are often useful when you want to vary a number by a small random amount.

positive and negative sides, the

Not all programming languages support normally distributed random numbers, however. The functions that support these PRNGs are listed here.

```
C#
    Uniform: Random.NextDouble
    Normal: NA
C/C++
    Uniform: rand
```

Uniform: rand
Normal: NA
Java

Uniform: Random.NextDouble

Normal: Random.nextGaussian
Python
Uniform: random.random
Normal: random.randn

R
Uniform: runif
Normal: rnorm

If your language does not support normal distributions, you can use the Box Muller transformation to transform uniformly distributed random numbers into normally distributed random numbers. Box Muller is discussed at length later in this chapter.

Roulette Wheels

Another popular random number technique is called the roulette wheel (Back, 1996). This technique only bears a slight resemblance to an actual roulette wheel, as seen in a casino. Roulette wheels are useful when you would like to choose between three or more categories. For example, consider if you wanted to create a robot to randomly explore a grid and your robot can perform only the following three actions:

- Move forward
- Turn left
- Turn right

Although the robot moves randomly, you might not want an even distribution among these three directions. You might want the robot to move as follows:

- Move forward (80% of the time)
- Turn left (10% of the time)
- Turn right (10% of the time)

Such a random number generation is relatively easy to implement. You must order these choices so that they each share part of the 0 to 1 range that a uniform PRNG will generate numbers for.

If \mathbf{x} is the random number, then the

if 0 < x < 0.8 then move forward if 0.8 < x < 0.9 then turn left if 0.9 < x < 1.0 then turn right

following list defines our actions.

The first line is needed because x will be below 0.8 in 80% of the cases. The second line is needed because x will be between 0.8 and 0.9 in 10% of the cases. Likewise, x will be between

0.9 and 1.0 in 10% of the cases.

PRNG Algorithms

There are many different PRNG algorithms. Often, there is a tradeoff between execution speed and randomness. Some algorithms are simply better than others. In this section, we will review some of the PRNG algorithms. Finally, we will review the Box Muller transformation. Box Muller is not a PRNG algorithm, but it can take the output of a uniform PRNG algorithm and produce normally distributed random numbers.

Performance is another very important consideration for PRNG selection. Most AI algorithms require a

Random number generation can thus be a very important consideration that affects the overall efficiency of the algorithm.

It is not critical that you understand

very large quantity of random numbers.

how all of the PRNG algorithms function internally. You can make use of the random numbers generated by an algorithm without learning the algorithm's internal details.

The PRNG algorithms covered in this book are as follows:

- Linear Congruential Generator (LCG)
 - Multiply With Carry (MWC)
 - Mersenne Twister

Different programming languages will use different PRNG algorithms. If your programming language does not use the algorithm you desire, the algorithm can be implemented separately in that language.

Linear Congruential Generator

The Linear Congruential Generator

Section 3.2.1. (Knuth, 1997). LCGs should not be used for applications

(LCG) is one of the oldest and most common PRNG algorithms in use. LCG is the built-in PRNG for C/C++, Java, and C#. LCG is documented in Donald Knuth's The Art of Programming,

needed. LCG is not typically useful for a Monte Carlo simulation because of the serial correlation. Serial correlation is the relation of a variable to itself over time. This means LCG random numbers are not high quality, nor are they suitable for cryptographic applications.

where high quality randomness is

implement and understand. It is implemented through a linear function clipped into a defined period. The equation for LCG is shown in Equation 4.2.

LCG is straightforward to

Equation 4.2: Random Numbers in a Range

$$X_{n+1} = (aX_n + c) \pmod{m}$$

The variables and acceptable ranges for the above equation are defined as follows:

m, 0 < m, The modulus a, 0 < a < m, The multiplier c, 0 <= c < m, The increment \times 0, 0 <= \times 0 < m, The seed, or sta

The **seed** value is updated with each random number generated. For LCG, the next seed is the internal state. These random numbers will be integers. They can be converted into the 0 to 1 range by dividing the random numbers by the maximum integer that the algorithm can produce. The maximum integer produced will depend on the

settings of **m**, **a**, and **c**.

The values chosen for **m**, **a**, and **c**

will have a great impact on the randomness of the numbers generated by the PRNG. Typically, you should not choose values of your own for **m**, **a**, and **c**. Much research has gone into finding optimal values. Wikipedia has a very

various PRNGs.
http://en.wikipedia.org/wiki/Linear_cong

good summary of the values used by

I typically use the values used by the GCC compiler.

```
m = 2e31

a = 1103515245

c = 12345
```

While LCG is a very commonly used PRNG, the Mersenne Twister is often a better alternative.

The Multiply with Carry (MWC)

PRNG was invented by George Marsaglia for the purpose of generating

Multiply with Carry

sequences of random integers with large periods. (Marsaglia, 1991) It uses an initial seed set from two to many thousands of randomly chosen values. The main advantages of the MWC method are that it invokes simple computer integer arithmetic and leads to very fast generation of sequences of random numbers. MWC has immense

periods, ranging from around 260 to 2 to the power of 2000000.

MWC works somewhat similarly to

LCG. Assuming 32 bit registers, LCG

uses only the lower 32 bits of the multiplication (Equation 4.2). MWC makes use of these higher bits through a carry. Additionally, multiple seed values are used. These seed values are typically created with another PRNG

We must first define a variable **r** to describe the "lag" of the MWC. We must provide a number of seed values equal to **r**. Like the LCG algorithm (Equation 4.2), we also have a modulus and a

multiplier. However, there is

algorithm, such as LCG.

increment in this case. The equation used to generate the random integers for MWC is shown in Equation 4.3.

Equation 4.3: Calculate Random Integer (MWC)

$$x_n = (ax_{n-r} + c_{n-1}) \mod b, \ n \ge r$$

The multiplier is represented by **a**, while the modulus is represented by **b**. There is an additional variable **c**, which represents the carry. The calculation for the carry is shown in Equation 4.4.

Equation 4.4: MWC Calculate C

$$c_n = \left| \frac{ax_{n-r} + c_{n-1}}{b} \right|, n \ge r$$

number in the sequence you are calculating. It is important that **n** always be greater than **r**. This is because the **x** values before **n** are the seed values, and we have **r** seeds.

Equation 4.4 is very similar to 4.3,

The variable **n** represents the

but while 4.3 uses the modulus operator to return the remainder, 4.4 actually carries out the division. We then use the floor of this result as the carry. The floor is the largest integer part of a number. For example, the floor of 7.3 would be 7. However, the floor of -7.3 would be -

The reason that we use the **floor** operator in Equation 4.4 is to ensure an

8. The floor of -7 would be -7.

the floor operator is given to make Equation 4.4 mathematically correct. The code examples for MWC do not make use of a call to the **floor** function.

The MWC generator has a much

integer result. Typically these operations are carried out on integer variables so

larger period than LCG, and its implementations are typically very fast to execute. It is an improvement over LCG, but it is not a commonly used generator. It is not the default random number generator for any computer language that I am aware of.

Mersenne Twister

The Mersenne Twister is a PRNG

quality pseudorandom integers. The Mersenne Twister was designed specifically to address many of the flaws found in older algorithms. (Matsumoto, 1998)

The Mersenne Twister is a very popular PRNG. It is the "built in" PRNG

developed in 1997 by Makoto Matsumoto and Takuji Nishimura. It provides for fast generation of very high

for Ruby, Python, and R. This book's examples also contain implementations for other languages. The Mersenne Twister algorithm creates high quality random numbers suitable for Monte Carlo simulations. Mersenne Twister is not a cryptographically secure generator.

However, its execution speed and high quality randomness make it a very attractive generator for AI.

The name Mersenne Twister comes from the fact that that the period of the Mersenne Twister is always chosen to be a Mersenne prime number.

A prime number is any number that can only be divided evenly by itself and one. For example, 5 is a prime number. A Mersenne prime number is any number **n** where **M** is also a prime number, as seen in Equation 4.5.

Equation 4.5: Mersenne Prime Numbers

 $M_n = 2^n - 1$

To see how this works, consider 5, which is a Mersenne prime number.

```
2^5 = 32
32 - 1 = 31
```

2 3 5

The number 31 is prime, so the number 5 is a Mersenne prime number. You can find a list of the known Mersenne prime numbers at the following URL.

http://en.wikipedia.org/wiki/Mersenne_p

Some other Mersenne primes are shown below.

```
17
19
31
61
89
107
127
521
607
1,279
2,203
2,281
3,217
4,253
4,423 (Wikipedia, 2013)
     The Mersenne Twister algorithm's
implementation is much more complex
than the algorithms already described in
this chapter, and a full description of it
```

is beyond the scope of this book. The

13

implementation of the Mersenne Twister based on the original C implementation provided by Matsumoto. One of the more tricky aspects of implementing the Mersenne Twister is

code examples do contain an

that it relies on bit shifts. This can be tricky for languages that do not support unsigned numbers. Java's non-support of unsigned numbers makes a Java implementation particularly tricky. For other languages, it is important to make sure that the variable sizes match the original C code.

Box Muller Transformation

Not all programming languages

might also be using a custom PRNG not provided by your programming language. There is an algorithm that can transform a continuous random number distribution into a normal one. This algorithm is called the Box Muller Transformation. (Box, 1958) The following pseudo code can be used to transform regular continuous random numbers into normal random numbers. (Ross, 2009) The Box Muller Transformation generates numbers two

at a time. To keep track of the pairs, we will place the two numbers into y1 and y2. We will use the variable useLast to

support the generation of random numbers in a normal distribution. You be used. The variable y1 will ultimately be returned, so if useLast is set to true, then move y2 into y1.

if (useLast)

track if there is a value in y2 waiting to

```
useLast = false;
} else
{

Begin by generating x1 and y1, both
in the range -1 to 1. Because rand()
```

y1 = y2;

normally returns 0 to 1, we scale **x1** and **y1**. We then square and sum both **x1** and **y1**, giving **w**. We continue until we have a **w** that is greater than or equal to 1.0.

do

```
x1 = 2.0 * rand() - 1.0;
x2 = 2.0 * rand() - 1.0;
w = x1 * x1 + x2 * x2;
} while (w >= 1.0);
w= sqrt((-2.0 * log(w)) / w);
Box Muller works by calculating two independent uniform distributions,
```

stored in x1 and x2. A scaling factor w is calculated across them; it allows x1 and x2 to be converted into a normally distributed random number. y1 = x1 * w;

```
useLast = true;
}
We scale both x1 and x
```

y2 = x2 * w;

We scale both x1 and x2, storing the results in y1 and y2.

return Y1;

We immediately return y1 and set

we immediately return y1 and set useLast to true. The next call to the function will return y2.

Estimating PI with Monte Carlo

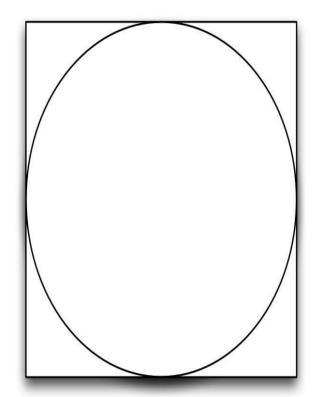
Monte Carlo algorithms attempt to estimate through random sampling, as it can be time intensive to calculate the actual value. Monte Carlo makes use of random samples to generate a good estimate. There are many different Monte Carlo techniques, some of which are hybrids between Monte Carlo and other techniques. (Robert, 2005) Later in this book, we will learn a Monte Carlo

One simple example of Monte Carlo is its estimation of the value of PI. Figure 4.4 shows a circle perfectly

method called Simulated Annealing.

inscribed inside of a square.

Figure 4.4: A Circle Inscribed in a Square



inside of the square and circle. The ratio of points inside to outside will tell us the value of PI. The area of the square is its length multiplied by its width. Because a square has the same width as length, the area of the square is essentially the width times itself, or width squared.

A circle's area is PI times its

We will now place random points

radius squared. The diameter of the circle is the same as the width of the square. We will calculate the ratio of the area of the circle to the square by using Equation 4.6.

Equation 4.6: Ratio of a Square and Circle

$$p = \frac{\pi r^2}{(2r)^2} = \frac{\pi}{4}$$

The width of the square is the same as two times the circle's radius. So we can describe the square's diameter as two times the radius squared. We will take the ratio of points inside the circle to outside and multiply by 4. This will give us an approximation of PI.

The pseudo code to produce this is shown below.

```
tries = 0;
success = 0;
for i from 0 to 10000
{
   // pick a point at random.
   x = rand();
   y = rand();
   tries = ties + 1;
```

```
// was the point inside of a cir
 if (x * x + y * y \le 1)
 {
 success++;
pi = 4 * success / tries;
    As we consider more points we
gain a more accurate approximation of
PI.
```

Chapter Summary

Random numbers are very useful to AI programs, particularly Monte Carlo simulations. A number of different random number generation algorithms exist. All are called pseudorandom number generators (PRNG). These random number generators vary in their ability to produce quality random numbers.

Some PRNGs are said to be cryptographically secure (CSPRNG). A random number generator may produce high quality random numbers, yet not be cryptographically secure. CSPRNG implies that the internal state of the

is not necessary to have a CSPRNG for AI applications. For AI, we are primarily interested in obtaining high quality random numbers and less interested in ensuring that these numbers do not reveal the internal state of the algorithm.

algorithm cannot easily be guessed by observing the output of the algorithm. It

One of the earliest and most common PRNG algorithms is the Linear Congruential Generator (LCG). While LCG can produce decent random numbers, the quality is not good enough for Monte Carlo simulations. Multiply with Carry (MWC) was created to overcome some of the limitations of LCG. The Mersenne Twister algorithm

A Monte Carlo simulation estimates a large problem by sampling small pieces of it. In this chapter, we saw that we could estimate PI using Monte Carlo. We looked at a circle that

was perfectly inscribed inside of a square. We randomly chose points and

quickly produces high quality random numbers. Mersenne Twister is acceptable for a Monte Carlo

simulation.

determined what points were inside of the circle and what were not. The ratio of these two point sets told us the value of PI.

The last two chapters introduced distance calculation and random numbers. The next chapter will show us

an algorithm that combines both techniques. It will show how observations can be divided into similar groups based on their distances from each other. K-Means clustering is one common technique for performing such divisions.

Chapter 5: K-Means Clustering

- Clustering
- Centroid
- Unsupervised Training
- K-Means

In previous chapters we saw that the input to a machine-learning algorithm is typically a vector of floating point numbers. Each of these vectors is called an observation, while the individual numbers that make up the vectors are called features. In this chapter we will learn about clustering. Clustering is the process of placing together observations with similar features, and thereby creating a cluster.

Clustering is a very useful means of

number of groups. Most clustering algorithms require you to specify the number of groups beforehand. Some clustering algorithms can automatically determine an optimal number of groups. This chapter focuses on the K-Means algorithm.

breaking observations into a specified

The process of clustering a finite number of observations into a specified number of clusters is called NP-Hard. NP-Hard is an abbreviation for nonproblems that cannot be solved via a brute force search, when there are simply too many different combinations to search every potential solution to a

problem. Clustering a non-trivial number

Informally, NP-Hard can be defined as

polynomial-time.

deterministic

K-Means makes use of random numbers to search for an acceptable clustering arrangement for the observations. Because the algorithm is based on random numbers, K-Means is said to be pendeterministic. This means

based on random numbers, K-Means is said to be nondeterministic. This means that multiple runs of the K-Means algorithm will result in different assignment of observations to clusters.

The opposite of a nondeterministic

Deterministic algorithms always produce the same output, given consistent input. Nearly all of the algorithms presented in this book are nondeterministic.

Clustering can be used both

algorithm is a deterministic algorithm.

independently and as a component to a larger machine-learning algorithm. Independently, clustering can be used to place similar items into groups. For example, you may have a large amount of observations that represent the buying habits of individuals. If each observation represents a customer, customers can be clustered. This allows you to make suggestive sales to customers based on what other customers in the same cluster

have purchased.

Genetic algorithms that use speciation often make use of clustering

as a component of the genetic algorithm. Genetic algorithms find solutions following a process that is loosely modeled after Darwinian evolution. (Banzhaf, 1998) Potential solutions to a problem compete with each other and reproduce to create potentially better solutions that carry the desirable traits from the parents. Often it is desirable to break the potential solutions into species and only allow breeding within a species. Because the potential solutions

species. Because the potential solutions are often vectors, K-Means can be used to speciate the potential solutions. (Green, 2009)

around, in various forms, since the 1950s. This algorithm has gone through a number of revisions by various researchers. James MacQueen first used the term "K-Means" in 1967. The actual idea for K-Means goes back to Hugo Steinhaus in 1957. Stuart Lloyd first proposed the standard algorithm in 1957 at Bell labs. However, his work wasn't published outside Bell labs until 1982. In 1965, E. W. Forgy published essentially the same method, which is why it is sometimes referred to as the Lloyd-Forgy algorithm. A more efficient version was proposed and published in Fortran by Hartigan and Wong in 1975 and revised in 1979.

The K-Means algorithm has been

Understanding Training Sets

Sets of observations are usually grouped into large collections called training sets. This data is used to train the machine-learning algorithm. Training is the process where the machine-learning algorithm is modified so that the output from the algorithm provides the desired information.

There are two very broad classes of machine learning algorithm that take very different types of training sets. Training is either supervised or unsupervised. When performing unsupervised training, you provide the

algorithm with an input observation as a vector. However, you do not specify an output vector that represents the expected, or ideal, output. Clustering is a type of unsupervised training.

Unsupervised Training

Recall the iris data set used in previous chapters? The iris data set has been applied to many different machine-learning algorithms. It can be used for both supervised and unsupervised training. This section shows how the iris data set can be applied to both.

First, we will take a look at how we would present the iris data set for

ratio observations about the dimensions of the iris petals. Additionally, the species of the iris is specified. Listing 5.1 shows a sampling from the iris data set.

unsupervised clustering. Recall that the iris data set consists of four individual

Listing 5.1: Several Rows from the Iris Data Set

5.1,3.5,1.4,0.2,Iris-setosa

- 4.9,3.0,1.4,0.2,Iris-setosa ... 7.0,3.2,4.7,1.4,Iris-versicolor
- 6.4,3.2,4.5,1.5,Iris-versicolor
- 6.3,3.3,6.0,2.5,Iris-virginica 5.8,2.7,5.1,1.9,Iris-virginica

For an unsupervised clustering, we would most likely use the first four measurements and ignore the species. We might tag the observations to the species, perhaps for later comparison. However, the clustering algorithm does

not need to know the species, because this is unsupervised training. The algorithm will not aim to determine what species the iris is, but will rather place the observations into clusters based on similarities among the observations.

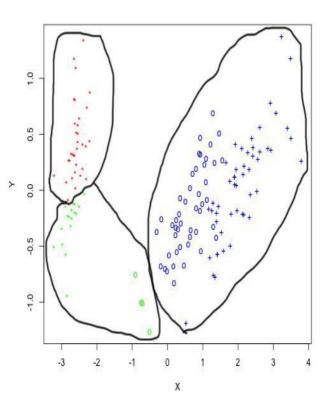
It is also important to note that it is not necessary to normalize the four observations. K-Means clustering does not inherently require normalization. Some other algorithms will require optional. You should only use clustering with K-Means if one or more of the features are so large that it might overwhelm the others. The four ratio features of the iris data set are all reasonably close in value, so K-Means clustering is not necessary in this case.

normalization, of course. For clustering the iris data set, normalization is

The iris data set does not have enough information expressed in the four ratio features to properly cluster it by species. This is okay. For clustering, we are really trying to visualize how close observations are and what clusters they might fall into.

Figure 5.1 shows one attempt to cluster the iris data set.

Figure 5.1: Iris Data Set Clustered



show what Figure 5.1 depicts, as there is quite a bit going on in this graph. The clusters are shown by color. They are also circled, for the benefit of those viewing this in black and white media. You can see that there are three clusters: red, green, and blue.

Each point is designated one of

It will take some explanation to

three total characters, which are pluses, asterisks, and O's. The character type indicates the species, as specified by the file in Listing 5.1. If the clustering algorithm were able to correctly cluster the iris species, each character of the same type would be the same color. If you look at Figure 5.1, you will see that this is not the case.

While you can see that the clusters are clearly defined, they do not line up with the species. This is mostly unavoidable. K-Means will sometimes come closer to picking the species, due

to its random nature. However, if you look at Figure 5.1, you will see that two regions are linearly separable. This means you could draw a line between them. However, two of the iris species are not linearly separable. There is overlap. It would be impossible for unsupervised clustering alone to find the separation between these two species.

You may be wondering how the four dimensional iris vectors were drawn on a two dimensional graph. I used R to reduce the dimensions to two

for graphing purposes. Dimension reduction is a common technique for data visualization, and was done using R's **cmdscale** function.

Supervised training is more

Supervised Training

restricted than unsupervised. A supervised training set consists of pairs of input and ideal output data. For the iris data set, you would input the four ratio measurement observations as a four dimension input vector. You would likely use one-of-n encoding to encode the species data into an ideal output vector. The machine-learning algorithm would be rated on how well it produced

the expected output vector, given the input vector. We will use supervised training with the iris data later in this book.

Understanding the K-Means Algorithm

The K-Means algorithm is relatively simple to implement. It works by assigning observations into a set number of clusters. There are three distinct steps to the K-Means algorithm: (Russel, 2009)

- Initialization Step
- Assignment Step
- Update Step

There are two different means by which the initialization step can be accomplished. (Hamerly, 2002) These

two initialization methods will be covered after we cover the other two steps. For now, just assume that the observations are initially assigned to the clusters by some means.

Assignment Step

The assignment and update steps are repeated until no observation moves to a new cluster. Each cluster is defined by two aspects. The first is its centroid, which is a vector of the same length as the observation. It is essentially an observation itself, but in fact represents the average of all observations inside the cluster. The centroid is thus essentially the point that is at the center of all observations in a cluster. In addition to a centroid, each cluster holds a list of observations assigned to that cluster.

The assignment step loops over all of the observations and assigns them to the cluster that has the nearest centroid. By nearest, I mean the shortest distance between the two vectors. Typically, the Euclidean distance is used; however, any of the distance algorithms from the last chapter would work.

It is also important for the update step to keep track of whether any observation moves from one cluster to another. This allows the K-Means algorithm to know when the algorithm is complete. If no observations move to a new cluster, then the K-Means algorithm is considered complete.

The pseudo code for the assignment step is shown here. First, we set a variable named **done** to **true**. We start out assuming that we are done. If any observation is reassigned from one cluster to another, we will set **done** to **false**.

done = true

We must now check each cluster and determine whether that cluster's observations might need to be moved to another cluster. We do not keep a list of observations; the observations "live"

foreach (cluster in clusters) {

inside of clusters.

We now loop over every observation in the current cluster and reassign if necessary.

```
foreach(observation in cluster)
{
```

Find what cluster is currently closest to the observation. The **findNearestCluster** function simply finds the minimum Euclidean distance between the current observation and the centroids of all the clusters.

targetCluster = findNearestClust

current cluster, then a move must occur. Perform the move and record that we are not done by setting **done** to **false**.

if (targetCluster != cluster)

If the targetCluster is not the

```
cluster.remove(observation);
  targetCluster.add(observation);
  done = false;
}
}
return done;
```

Finally, return the value of done so that the rest of the program can decide if it should continue iterating or exit.

Update Step

step. Like many machine learning algorithms, K-Means is iterative. The training process goes through a large number of iterations, and every iteration should see some gradual improvement. At some point, each iteration brings little or no improvement. This is when an iterative algorithm stops. The real work of the update step is

to recalculate the centroids for each of the clusters. During the previous assignment step, it is likely that the contents of each cluster were changed.

The update step is executed after

the assignment step. These two steps keep cycling until there no observations change clusters during the assignment need to calculate a mean vector of four dimensions. This mean becomes the centroid for the cluster.

5.1, 3.5, 1.4, 0.2, Iris-setosa
4.9, 3.0, 1.4, 0.2, Iris-setosa
7.0, 3.2, 4.7, 1.4, Iris-versicolor

This vector would be calculated as

follows:

Because of this, the centroid for each cluster may have become invalid. To account for this, we need to recalculate each cluster's centroid, which is a matter of simply calculating the mean of each feature of the observation. For example, if the following three iris flowers were all in a cluster, we would

Which results in the following centroid:

[5.7, 3.2, 2.5, 0.6]

element1 = (5.1 + 4.9 + 7.0) / 3

element2 = (3.5 + 3.0 + 3.2) / 3element3 = (1.4 + 1.4 + 4.7) / 3element4 = (0.2 + 0.2 + 1.4) / 3

Of course, as discussed previously, the iris species column is not used by the algorithm.

Initializing the K-Means Algorithm

In the last few sections we saw how the assign and update steps were performed. Both of these operate on clusters that already have observations assigned to them. We must therefore start in a state where observations are assigned to clusters.

In this section we will look at two different means of initializing the clusters randomly. The initialization step of K-Means is stochastic, or random. The update and assign steps are both deterministic. However, because the algorithm has a non-deterministic

deterministic.

There are two very popular means of initializing the K-Means algorithm:

beginning, the entire algorithm is non-

the Random algorithm and the Forgy algorithm. The name of first method — "Random"—is a bit misleading, however, as both algorithms use random numbers.

Random K-Means Initialization

The random algorithm is very simple. You simply create the requested **K** number of clusters and assign random observations to each of these clusters. It

created clusters. First, we calculate the number of dimensions the observations have. The K-Means algorithm requires that each dimension contain the same number of

is also important that we do not let any cluster have zero observations. Of course, K should never be higher than the number of observations. That is, you cannot cluster 30 observations into 50 clusters. It is also very important that the "random" initialization proceed directly to the update step. This allows the centroids to be calculated for the newly

dimensions. This is simply the array length.

dimensions = theObservations.leng

Next, we must create \mathbf{K} clusters. We loop from zero up to, but not including \mathbf{K} .

```
for i from 0 to K
{
  clusters.add(new Cluster(dimens:
}
```

We must now assign each of the observations to a random cluster. First, loop over all observations provided.

Then, pick a random cluster. Assign

foreach (observation in theObserv

a random integer between 0 and **K-1**. Add that observation to the cluster.

```
clusterIndex = randInt(K);
cluster = clusters[clusterIndex]
cluster.add(observation);
```

We can now handle any clusters that might have no observations assigned to them.

```
foreach (cluster in this.cluster:
{
  if (cluster.length == 0)
  {
```

It is time to add one observation to this cluster. We do not want to create another zero length cluster in the process of fixing this cluster, however. Find a random cluster that has more than one observation already. Make sure that the chosen cluster is not the same cluster as that we are trying to fill.

Once we find the cluster, we can move the observation. Choose a random observation from the source cluster and move it to the empty cluster. We can now set the **done** flag to **true**.

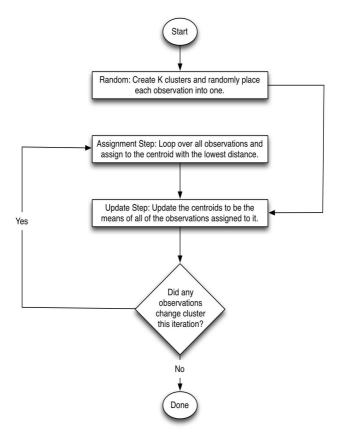
```
sourceObservationIndex = rnc
sourceObservation = source[s
source.remove(sourceObservation)
cluster.add(sourceObservation)
```

```
done = true;
}
}
}
updateStep();
```

Once the observations have been assigned to their clusters, we can perform the update step.

Figure 5.2 shows the flow chart for a K-Means algorithm that uses random initialization.

Figure 5.2: Random Initialization



initialization step already assigned the observations to clusters. You will see in the next section that the for Forgy K-Means initialization has a slightly different flow. K-Means **Forgy Initialization** Forgy initialization works by first

establishing the centroid values and then assigning the observations to the nearest clusters. This is done using the pseudo

Note that the random initialization

make sense, because the

goes directly to update form initialization. Performing the assignment step after a random initialization would dimensions = theObservations.leng
usedObservations = new HashSet();
We now loop through and create K
clusters.

Create the cluster, with the correct

either.

for i from 0 to K

code described below. First, determine the number of dimensions in the observations. Each observation should have the same number of dimensions. We will also keep a hash set of **usedObservations**. We will not use every observation for initialization, but we do not want to reuse an observation,

cluster = new Cluster(dimension:

number of dimensions.

clusters.add(cluster);

With the cluster created, select a random observation. Do not choose an observation that has already been used.

```
observationIndex = -1;
while (observationIndex == -1)
{
  observationIndex = randInt(the
  if (usedObservations.contains
  {
    observationIndex = -1;
  }
}
```

Now we have a randon

used. Create a cluster with only that observation and assign that observation to the cluster's centroid.

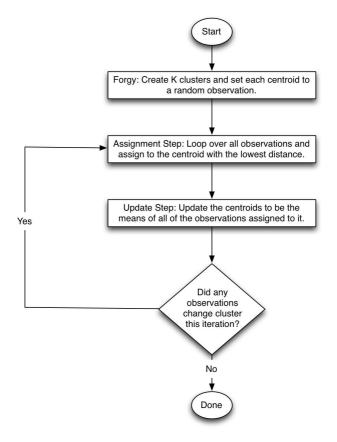
observation = theObservations[ol

observation that was not previously

rigure 5.3 shows the flow of an

application that uses Forgy initialization.

Figure 5.3: Forgy Initialization



As you can see from the above figure, the assignment step is processed right after the initialization step. This is because Forgy has already set up the cluster centroids, and we now need to assign all of the observations to the clusters.

Chapter Summary

Clustering is a method for placing observations into clusters. The similarity between observations determines what observations are placed into what clusters. Clustering is an example of unsupervised training.

There are a number of different algorithms for clustering. One of the most popular is the K-Means algorithm. The K-Means algorithm assigns the observations into a fixed number of clusters. It takes several iterations for K-Means to move all of the observations into acceptable clusters. You should iterate the K-Means algorithm until you

changes clusters.

There are three different steps that are used in the K-Means algorithm. The

have an iteration where no observation

initialization step creates the initial clusters. The assignment step updates the centroid for each cluster. The centroid is the vector average of all observations assigned to that cluster. The update step

recalculates all centroid values based on observations assigned to those clusters.

This chapter introduced you to clustering and unsupervised training. In the next chapter, you will learn about

error calculation. Error calculation is primarily used in supervised training. It helps to calculate the difference between the actual output and the ideal output of a



Chapter 6: Error Calculation

- Supervised Training
- Sum of Squares Error (SSE)
- Mean Squares (MSE)
- Root Mean Squares
- Data Sets

Error calculation is very important for supervised training. A training set for supervised training consists of vector pairs. These pairs align input vectors with an output, or ideal, vector that is the expected response to the provided input vectors.

Listing 6.1 shows an example of how vector pairs would be constructed for the XOR function.

Listing 6.1: The XOR Function/Operator

```
Input: [0,0]; Ideal: [0]
Input: [0,1]; Ideal: [1]
Input: [1,0]; Ideal: [1]
Input: [1,1]; Ideal: [0]
```

The XOR function always returns **true** when the two inputs are different. If the two inputs are the same, then it returns **false**. In the above listing, **true** is normalized to 1 and **false** to 0. The above training set would be used to teach a machine-learning algorithm to

emulate the XOR function. This is a common introductory task for machine learning algorithms.

In the above listing, there are two inputs: 0 and 1. The ideal output for each of the four input vectors is also provided. This training set contains four input/ideal output pairs.

There are a variety of different error calculation methods that are commonly used with machine learning algorithms. In this chapter we will look at the following three error calculation methods:

• Sum of Squares Error (SSE)

- Mean Square Error (MSE)
- Root Mean Square Error (RMS)

The most commonly used error calculation method is Mean Square Error (MSE). However, this does not mean the MSE should always be used. Sometimes, the machine-learning algorithm in use will dictate the error calculation method that you should use. You can also use multiple error calculation methods if necessary, for comparison.

The following sections will describe each of these error calculation methods.

Sum of Squares Error

The Sum of Squares Error (SSE) is a very simple error calculation method used by some machine learning algorithms. A high SSE value indicates that there is a large difference between the expected output and the actual output. A training algorithm should work to minimize SSE.

The calculation of SSE is shown in Equation 6.1. (Draper, 1998)

Equation 6.1: Sum of Squares Error (SSE)

$$SSE = \sum_{i} (\hat{y}_{pi} - \bar{y_{pi}})^2$$

Where **y** hat is the ideal output and **y** bar is the actual output.

The most common reason to use

SSE is that some training algorithms require it. SSE is essentially the sum of squares of the individual variances of each output. Because of this, bigger training sets will always tend to have larger SSE values. This is one of the weaknesses of the SSE value—you

cannot directly compare the SSE values from two training sets of different sizes.

Root Mean Square

SSE method in that it is based on the squares of the individual differences between expected output vectors and the actual output. However, a mean is taken of all of these squares and then the square root is taken of this mean. Because the RMS is based on a mean, you can compare the RMS values of two different training sets. (Draper, 1998)

error calculation method is similar to the

The Root Mean Square (RMS)

Equation 6.2: Root Mean Square (RMS)

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2}$$

Where **y** hat is the ideal output and **y** bar is the actual output.

Mean Square Error

MSE error calculation is the most commonly used error calculation for machine learning. Most, but not all, Internet examples of neural networks, support vector machines, and other models make use of MSE. MSE is shown in Equation 6.3. (Draper, 1998)

Equation 6.3: Mean Square Error (MSE)

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - \bar{y}_i)^2$$

Where **y** hat is the ideal output and **y** bar is the actual output.

The mean square error is essentially the mean of the squares of the individual differences. Because the individual differences are squared, it does not matter to MSE if the difference is positive or negative.

You may be wondering how to choose between RMS and MSE. RMS and MSE are very similar. One important difference is that RMS is linear whereas MSE is not. If you were to double every error in the training set, the RMS errors would also double, while the MSE errors would not. Sometimes it is useful to be able to compare errors like this.

Comparison of Error Calculation Methods

This section shows how to add random distortion to a training set. Listing 6.2 shows how small, medium. large, and huge distortions affect each of the training sets.

Listing 6.2: Error Calculation Methods			
Type	SSE	MSE	Rì

Small 0.01 2505

62634 0.251

1.002

100.216

Medium Large 250538 1 (Huge 25053881

The largest effect is on the SSE

error calculation, because SSE is a simple summation of the errors. SSE has a larger change than RMS. You can see that RMS is essentially the square root of RMS.

Partitioning Training Data

You typically do not want to use all

available data for training, as there is almost always noise in your data. The word "noise" is used to describe small distortions that are not consistently reproducible. A successfully trained algorithm will be able to see through the noise and still predict accurately. Over fitting occurs when the algorithm memorizes the noise. Because the noise

the algorithm's ability to recognize data outside of the training set. Because noise is not consistent, it will cause the algorithm to see false patterns. Such patterns create a phenomenon called training set bias.

is not consistent, this will greatly impair

Selection bias is another concern. If you need to choose from among several competing machine learning algorithms, you should not simply choose the algorithm that trained to the lowest error, or you will likely pick the most over fit model.

Available data is typically broken into three sets to avoid bias. It is important that these sets are randomly

available data in order to avoid bias. For time-series data, you select chronological ranges. The three sets that training data is typically divided into are listed here.

• Training set

Validation set

Test set

sampled from available data, as you do not want to introduce any bias when selecting the items for each set. Randomly select items from the

The training set is the data with which you train your algorithm. This is usually the largest of three sets. Training data is often selected as 80% of

test. It is important to remember that error on your training data is often very optimistic. This is because the training data was used to train the algorithm.

available data. You can then split the remaining 20% between validation and

If you are evaluating several different algorithms, you should use the validation set next to see what algorithms learned the best. Use data that the algorithms did not see during the training, as the algorithms should be unbiased to this data.

Chapter Summary

This chapter introduced supervised training, using data sets. A supervised data set is used with a supervised training algorithm and contains pairs of vectors. Each of these pairs represents one element in the training set. Each pair contains an input vector and an output vector that represents the expected output from that input vector. Machine learning algorithms are evaluated based on how closely the actual output matches the ideal expected output.

There are several different error calculation algorithms. One of the most basic is the Sum of Squares Error (SSE).

between the actual and expected outputs for the machine-learning algorithm. The SSE algorithm then squares and sums each of these differences.

This method calculates the difference

The Mean Squares Error (MSE) is one of the most commonly used distance calculation methods in machine learning. This calculation is similar to SSE; however, MSE is divided by the number of elements, thus producing an average.

Once you have selected your algorithm, you can use the test set to give you an idea of how well the algorithm might perform with real data. This should be the final indicator of the overall performance of your chosen model. MSE is not linear—if the

double.

The Root Mean Square (RMS) error is essentially the square root of the

difference doubles, MSE will not

This allows you to directly evaluate two RMS errors. If the difference between the actual and ideal vectors doubles, then RMS will also double.

MSE error. Unlike MSE, RMS is linear.

This chapter introduced several concepts in supervised training and described how to construct supervised training sets. It also discussed several methods for evaluating these data sets.

training sets. It also discussed several methods for evaluating these data sets. The next chapter introduces machine learning. You will see how simple models can be constructed and trained to produce the correct output.

Chapter 7: Towards Machine Learning

- Training a Polynomial
- Greedy Random Training
- RBF Functions
- RBF Network Model

In previous chapters we saw that a machine-learning algorithm typically accepts an input vector and produces an output vector. To transform this input vector into an output vector, two additional vectors can be used. These additional vectors are referred to as long-term and short-term memory. Long-

term memory can also be referred to as weights or coefficients. It is adjusted through training. Short-term memory is not used by all machine-learning algorithms.

It might be helpful to think of a

machine-learning algorithm as a function. We will treat a very simple equation as though it were a machine-learning algorithm in equation 7.1, in order to demonstrate.

Equation 7.1: Simple Linear Equation

f(x) = 5x

Here we think of **x** as a single value—a scalar, rather than a vector. The value 5 is a coefficient. Coefficients are

into Equation 7.1 and evaluate the results. **Listing 7.1: Simple Training Data** Input: [1], Desired Output: [7] Input: [2], Desired Output: [14] Input: [3], Desired Output: [21] The coefficient of 5 would not

usually grouped into a vector and represent the long-term memory of the algorithm. When we train Equation 7.1, we will adjust the coefficient until we arrive at a value that produces the desired output. If Listing 7.1 represented the training data for the algorithm of Equation 7.1, we could feed the input

provide the desired output. As we saw

in Chapter 6, we could calculate the error between the above desired outputs and the actual outputs provided in Listing 7.1. For example, the input of 1 to Equation 7.1 would produce 5, while our desired output for 1 is 7.

There are many different ways to find a suitable coefficient for machine learning algorithms. Coefficient adjustment methods is one of the primary areas of research for machine learning.

If the machine learning algorithm is a linear function, as is the case with Equation 7.1, mathematical techniques can often be used to find a suitable coefficient. For this simple case, we only need to find the coefficient that coefficient would be 7. A coefficient of 7 also yields a zero error for the other training set elements.

Not all data sets will be so easy. In

yields 7 when multiplied by 1. This

fact, it is extremely rare to fit the coefficients (or long-term memory vectors) to result in an error that is exactly zero. This is because most data contains noise. Noise is any outcome that is not consistently reproducible given its input data, and thus contributes to a higher error rate. Because of noise, the goal of a machine learning algorithm is usually for the algorithm to perform well on new data, rather than displaying zero error.

If you do get a zero error, you

data. At this point, the algorithm simply recalls memorized input vectors rather than learning to abstract output. An over fit algorithm will not perform well on new data that is not in the original training set.

We will now look at some methods

should be suspicious that your coefficients are over fit. Over fitting occurs when the machine learning method has memorized your training

for optimizing the coefficients to lower the error and be introduced to a few foundational algorithms for optimizing the coefficients. The next chapters will discuss more advanced algorithms, such as simulated annealing and Nelder Mead. in this book are generic. Given any longterm memory vector, these algorithms can attempt to optimize. This is not the case with every training algorithm, however. Some training algorithms use specific insights into the algorithm that they are trying to train. We will see such algorithms in Chapter 10. However, most of the algorithms in the other chapters of this book are generic.

Most training algorithms presented

Coefficients of a Polynomial

This section describes how to implement a generic training method in order to optimize the coefficients of a polynomial. We will use the polynomial as the machine-learning algorithm that we seek to optimize. Typically, you will optimize the coefficients into something more complex than a simple polynomial, but this example will serve as a great introduction to machine learning. Fitting a polynomial to a dataset illustrates the fundamentals of how more complex machine learning algorithms work.

A polynomial is a mathematical expression consisting of variables and

constant coefficients and uses only the operations of addition, subtraction, multiplication, and positive integer exponents. Equation 7.2 shows a typical, third degree polynomial. (Lial, 2010)

Equation 7.2: A Third Degree

Polynomial

 $f(x) = 2x^2 + 4x + 6$ The above mathematical function

The input and output vectors for this function are both of size one. There are three coefficients in Equation 7.1: 2, 4, and 6. In this case, the coefficients are multiplied against the variable **x**. The coefficient 2 is multiplied against **x**

accepts a value x and returns a value y.

Technically 6 is multiplied against x to the power of zero. Though x to the power of zero is equal to one.

squared, the coefficient 4 is multiplied against x. Even 6 is a coefficient.

The above polynomial is said to be of the "third degree" because there are three terms. Each term relates to a coefficient. The three coefficients used in Equation 7.1 can be thought of as a vector and described as follows:

[2,4,6]

For Equation 7.1, the coefficient is already specified. Often we will need to use machine learning to determine what the coefficient(s) should be. To do so,

includes the expected outputs for a variety of inputs. Such data can be collected experimentally. In order to fit these observations to a third degree polynomial, we can use machine learning to help.

We will begin by creating some

you would use a training set that

training data. We already know that we want the solution to be the coefficients [2,4,6]. This is a completely contrived example, but it will demonstrate how to use some basic training algorithms. To generate the training data, loop over somex values and calculate the polynomial for each. Then, use random coefficients to train to the correct coefficients. We will use only the

correct coefficients. The generated training data is shown in Listing 7.2. As you can see, we

training data to see if we can rebuild the

loop the input from -50 to +50 and calculate the ideal output.

Listing 7.2: Polynomial Training Data

```
[BasicData:
                           input: [-
50.0], ideal:[4806.0]]
```

[BasicData: input: [-49.0], ideal:[4612.0]] [BasicData: 48.0], ideal:[4422.0]]

input: [input: [47.0], ideal: [BasicData:

[4612.0]]

[BasicData: input:[48.0], ideal: [4806.0]]

[BasicData:

input: [49.0], ideal:

Given the above data, we will now see how the coefficients can be adjusted to produce the above data. In the next section we will see how we can use the training data in Listing 7.2 to reconstruct the polynomial. Of course, we will assume that we did not know the actual polynomial in the first place. We only assume we have Listing 7.2.

Introduction to Training

There are many different ways to adjust the long-term memory of a machine-learning algorithm during training. In this section, we will look at greedy random training. This method is simple to implement. In the next chapter, we will look at more robust training algorithms. Robust training algorithms will typically find an optimal setting for long-term memory faster than greedy random training.

Greedy Random Training

Greedy random training is extremely simple to implement.

and always maintains the best vector seen so far. This algorithm is sometimes called a random walk.

This algorithm can be seen in the

Listing 7.3: Greedy Random Training

pseudo code shown in Listing 7.3.

(minimize score)

function iteration (

Essentially, all it does is randomly select values for the long-term memory vector. This algorithm is greedy in the sense that it only accepts a new memory vector if the new vector is an improvement over the previous one. This algorithm keeps choosing new random values for the long-term memory

```
ltm, // the current long term me
lowRange, // the lowest value to
highRange // the highest value to
// Score the current state.
oldScore = calculateScore(ltm);
// Keep a copy of the current st
// fail to improve it.
len = ltm.length;
oldLtm = ltm.clone();
// Set to a random state.
for i from 0 to len
ltm[i] = rand(lowRange, highRange
// Score the new random vector.
newScore = calculateScore(ltm);
// Greedy decision. Did the rand
// If not, then back it out.
if ( newScore > oldScore )
```

```
Ltm = oldLtm.clone();
}
```

The above code implements one iteration of a greedy random algorithm. There are three parameters that you pass to the above function.

- Parameter 1. The long-term memory vector that you would like to optimize.
 Parameters 2 & 3. The low and
- Parameters 2 & 3. The low and high ranges for the values that you would like to randomly assign to the individual elements in the long-term memory vector.

random values to the long-term memory vector. The score of the vector is compared to the score from before the randomization. If the vector's score did not decrease, then throw out the changes and revert to the previous vector. This is why it is called greedy. It will only accept improvements. This is not always the best policy. As the old saying goes, "sayating a part that are the

The iteration function then assigns

"sometimes you have to take one step backward to take two steps forward." Believe it or not, the greedy random trainer can actually train vectors. Running it against the polynomial (from Equation 7.2) yields the following results.

Iteration #999985, Score=37.93061 #999986, Score=37.93061 Iteration #999987, Iteration Score=37.93061 #999988, Score=37.93061 Iteration #999989, Score=37.93061 Iteration Score=37.93061 Iteration #999990, #999991, Iteration Score=37.93061 Iteration #999992, Score=37.93061 #999993, Score=37.93061 Iteration #999994, Score=37.93061 Iteration #999995, Score=37.93061 Iteration #999996, Score=37.93061 Iteration Iteration #999997, Score=37.93061 Iteration #999998, Score=37.93061 Iteration #999999, Score=37.93061 Iteration #1000000, Score=37.930 Final score: 37.93061791363337 2.0026889363153195x^2+4.057350732 As you can see, the greedy random training algorithm came reasonably

to the expected coefficients.

#999984,

Iteration

Score=37.93061

4.057, and 9.3933].

The greedy random algorithm is often used as a benchmark. You can

Instead of getting [2,4,6], we got [2.002,

compare the greedy random result against a new algorithm that you are evaluating. If the new algorithm does not outperform the greedy random algorithm, then you know the new algorithm is

performing very poorly.

Radial Basis Networks

In the last section we looked at how to optimize the coefficients for a polynomial. Most machine learning algorithms are much more complex than a simple polynomial. In this section we will introduce an RBF Network. (Bishop, 1996) The RBF network is a statistical model that can be used both for regression and classification.

There are many different methods for training an RBF network. The RBF network has a vector that represents its long-term memory. For an RBF network, the long-term memory is a combination of coefficients and other parameters.

for the RBF network. It can be trained by both greedy random and hill climbing algorithms, and is based on radial basis functions (RBF).

The next section will briefly

There is no short-term memory vector

review RBFs and describe the exact makeup of this vector.

Radial Basis Functions

Radial basis functions are a very important concept in AI, as many different AI algorithms make use of them. There are a number of different RBF types, several of which will be introduced in this chapter.

typically located somewhere along the x-axis. The RBF will reach its maximum value at the center. This maximum value is called the peak, and is often set to one. In the context of RBF networks, the peak is always set to one and the center varies accordingly.

symmetric about its center, which is

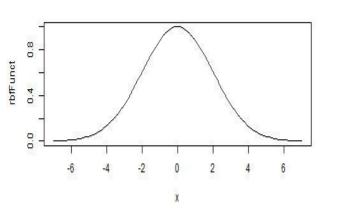
A radial basis function is

RBFs can have many dimensions. The output of an RBF will always be a single scalar value, regardless of the number of dimensions in the vector passed to the RBF.

There are a number of commonly used RBFs. We will start with the most common: the Gaussian function. Figure 7.1 shows a graph of a 1D Gaussian

function centered at 0.

Figure 7.1: Gaussian Function



RBF functions are commonly used to selectively scale something, and Gaussian is no different. Consider

Figure 7.1. If this function were used to scale something, you would have maximum intensity at the center. The intensity would fall off in either the positive or negative directions as you moved from the center.

Before we can look at the equation

for the Gaussian RBF, we must consider how to process the multiple dimensions. It is important to note that RBFs accept multi-dimensional input to return a single value. It does this by calculating the distance between the input and the center vector of the RBF. This distance is called r. The RBF center and input to the RBF must always have the same number of dimensions for the calculation to occur. Once we calculate r, then we

can calculate the individual RBF function. All of the RBF functions make use of this calculated **r**.

Equation 7.3 shows how to

equation 7.3 snows now to calculate **r**.

Equation 7.3: Calculating r

$r = ||\mathbf{x} - \mathbf{x}_i||$

The double vertical bars you see in the equation above represent that the function describes a distance. Euclidean distance is almost always used for an RBF. However, other distances might be

used for certain very specialized cases. The examples provided for this book always use the Euclidean distance. Therefore, **r** is simply the Euclidean

distance between the center and the x vector. The value r will be used in each of the RBF functions used in this section.

The equation for a Gaussian RBF is shown in Equation 7.4.

Equation 7.4: Gaussian RBF

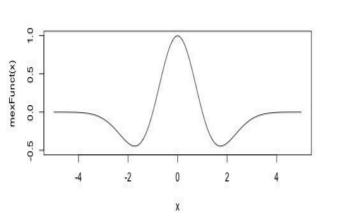
$$\phi(r) = e^{-r^2}$$

Once you've calculated r, it is fairly easy to calculate the RBF. The Greek letter PHI, which you see at the left of the equation, always represents an RBF.

The Gaussian is not the only RBF, and other RBFs have different shapes. If you are using the RBF to scale, these

different shapes can give you different ways to scale a number. Figure 7.2 shows the Ricker Wavelet.

Figure 7.2: The Ricker Wavelet (Mexican Hat Function)



as an RBF. It is often called the Mexican hat function, due to its pictorial resemblance to a sombrero. The equation for the Ricker Wavelet is provided in Equation 7.5.

Equation 7.5: The Ricker Wavelet

The Ricker Wavelet is often used

(Mexican Hat Function)

$$\phi(r) = (1 - r^2) \cdot e^{-r^2/2}$$

As you can see from Figure 7.2, the Ricker Wavelet actually scales negatively just at the edges, and then returns to zero.

Different RBF functions are useful in different situations. Some other common RBF functions include:

- Multiquadric
- Inverse quadratic
- Inverse multiquadric
- Polyharmonic spline
- Thin plate spline

We can make use of the RBF function to implement a statistical model called the RBF network. We will be able to train this model using any of the techniques discussed so far.

Radial Basis Function Networks

A Radial Basis Function network is

or more Radial Basis Functions, each of which receives the weighted input attributes used to predict the output. The following equation describes an RBF

a statistical model that can be used for both classification and regression. It provides a weighted summation of one

Equation 7.6: An RBF Network

network.

$$f(X) = \sum_{i=1}^{N} a_i p(||b_i X - c_i||)$$

Note that the double vertical bars above mean to take the distance. Such symbols do not specify what distance algorithm to use; this is your choice. In the above equation **X** is the input vector

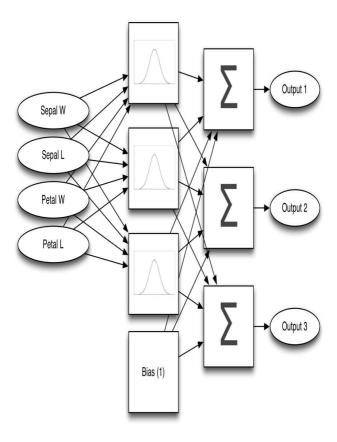
example), **a** is the vector coefficient (or weight) for each RBF, and **b** specifies the vector coefficient to weight the input attributes. We will see pseudo code for Equation 7.6 later in this chapter.

of attributes, **c** is the vector center of the RBF, **p** is the chosen RBF (Gaussian, for

RBF network to the iris data set. Figure 7.3 provides a graphic representation of this application.

In our example, we will apply the

Figure 7.3: An RBF Network for the Iris Data



describe each iris species. The above diagram assumes that we are using oneof-n encoding for the three different iris species. It would also be possible to use equilateral encoding and have only two outputs. To keep things simple, however, we will use one-of-n. We also choose to use three RBF functions. This is purely an arbitrary choice. Additional RBF functions allow the model to learn more complex data sets. However, more

The above network contains four

inputs (the length and width of petals and sepals), which map to the features that

Arrows represent all coefficients from the equation. The arrows between the input attributes and RBFs are

RBF's take more time to process.

and the summation are represented by a. You will also note that there is a bias box. This is a synthetic function that always returns a value of 1. Because the bias function's output is constant, no inputs are required. The weights from the bias to the summation function very similarly to the vector intercept in linear regression. Bias is not always bad! In this case it is an important component to the RBF network. Bias nodes are also very common in neural networks.

represented by **b** in Equation 7.6. Similarly, the arrows between the RBFs

Because there are multiple summations, you can see that this poses a classification problem. The highest summation specifies the predicted class.

If this were a regression problem, there would be single output. The single output would represent the predicted output for regression.

You will also notice that there is a

bias node in Figure 7.3. The bias node is located in the place where an additional RBF function might go. However, the bias node does not accept any input unlike an RBF. The bias node always outputs a constant value of one. Of course, this constant value of 1 is multiplied by a coefficient value. This has the effect of the coefficient always being directly added to the output, regardless of the input. Bias nodes are very useful when the input is zero, as

they allow the RBF layer to output

values even when the input is zero.

The long-term memory vector for

The long-term memory vector for the RBF network is made up of several different components:

- Input coefficients
 - Output/Summation coefficients
 - RBF width scalars (same width in all dimensions)
 - RBF center vectors

The RBF network will store all of these components as a single vector. This vector becomes the long-term memory of the RBF network. We will then make use of either greedy random or hill climbing training to set the vector to values that will produce the correct iris species for the features presented.

This model works almost exactly

like the polynomial that we saw before. The only difference is that the equation is much more complex, as we now must calculate several output values and RBF functions.

Implementing an RBF Network

This section outlines the pseudo

code for two major functions in the implementation of an RBF network. First, we will look at the function that initializes an RBF network. This

vector that is used for the RBF network. To create the RBF network, you must provide the following three pieces of information.

function allocates the long-term memory

- Input countRBF count
 - Output count

The input and output counts simply specify the sizes of the input and output vectors. Your data set will dictate these values. The RBF count is a bit more

values. The RBF count is a bit more subjective. The more RBF functions you have, the better the model will be able to predict desired outcomes. However,

using more RBF functions increases

inefficiency.

Listing 7.4 shows how an RBF

Listing 7.4: Initializing an RBF Network

network is initialized.

```
function initRBFNetwork(
  theInputCount, // the number of
  rbfCount, // the number of RBF:
  theOutputCount // the output cou
)
{
  result = new RBFNetwork();
  // set simple properties on the
  result.inputCount = theInputCount
```

// Calculate input and output we
// Add 1 to output to account for
inputWeightCount = inputCount *
outputWeightCount = (rbfCount +

result.outputCount = theOutputCo

```
rbfParams = (inputCount + 1) * :
// allocate enough space for the
result.longTermMemory = alloc(in
+ outputWeightCount + rbfParams)
// Set more properties on the ma
result.indexInputWeights = 0;
result.indexOutputWeights = inpu
// Allocate RBF functions
result.rbf = new FnRBF[rbfCount]
// Set up all of the RBF function
for i from 0 to rbfCount
  // The index for the current I
  rbfIndex = inputWeightCount +
  // allocate a Gaussian and spe
  // the location in long term r
  // function's parameters are :
  // the width, followed by the
  result.rbf[i] = new GaussianFi
    inputCount, result.longTerm1
// return the newly constructed
```

```
return result;
}
```

The method begins by allocating an object named **result** to hold the RBF Network. This object will hold the long-term memory and a few other basic items about the network.

The above code calculates exactly

how much long-term memory is needed to hold the coefficients and RBF parameters. The individual RBF functions are then allocated and pointed to the long-term memory for their parameters. The RBF parameters are their widths, followed by their center dimensions.

The above code does not actually

random values. This will give the RBF network an initial starting point. Training will refine the long-term memory values into useful values that produce output closer to the expected outputs. For the iris data, these are the outputs that define what species the network thinks the inputs correspond to.

Once the RBF network has been set

fill the long-term memory with any values. Once the network has been allocated, you will typically assign it to

up and the long-term memory has been set, the network is ready for training. We will call the RBF model and score how well the initial outputs match up. Of course, we are starting with random values, so the output will not be good. However, you have to start somewhere.

Just as was done for the

polynomial, we must calculate the output for the RBF network. The pseudo code in Listing 7.5 is provided to show the calculation in this context.

Listing 7.5: Calculating an RBF Network

function computeRBFNetwork(

```
input, // the input vector
network // the RBF network
)
{
  // First, compute the output val
  // Add one additional RBF output
  // to one).
rbfOutput = alloc(network.rbf.le
```

// Bias is always valued 1.

```
rbfOutput[rbfOutput.length - 1]
for rbfIndex from 0 to network.
{
  // weight the input
 weightedInput = alloc(input.le
  for inputIndex from 0 to input
    memoryIndex = network.index
    + (rbfIndex * network.input(
    weightedInput[inputIndex] =
      * network.longTermMemory[r
  // calculate the rbf
  rbfOutput[rbfIndex] =
 network.rbf[rbfIndex].evaluate
// Calculate the output, which :
// of the weighted result of the
result = alloc(network.outputCoi
for outputIndex from 0 to result
  sum = 0;
  for rbfIndex from 0 to rbfOut;
```

The above code calculates the final output in several layers. We create a variable named **rbfOutput**. As its name implies, it will hold the outputs from the RBF functions. We loop over all of the RBF functions and calculate the weighted input to the RBF. The weighted

input is simply a vector created by

vector is filled, except for the last element of the **rbfOutput** vector. The last element gets a 1 and functions as the bias node.

Once the **rbfOutput** vector has been filled, it is multiplied by the output coefficients. The output coefficients are represented by the vertical column of

arrows closest to the right in Figure 7.3. The calculated output values are placed into the result vector, and then the result

multiplying each input by that RBF function's input coefficients. On Figure 7.3, these are the coefficients represented by the vertical group of arrows closest to the left. As each RBF function is calculated, the **rbfOutput**

vector is returned to the calling function.

Using an RBF Network

Examples for using RBF networks with the iris data set, as well as the XOR data set, are provided below. These allow you to see how the RBF

network can be trained to learn the expected output for both XOR and iris. First, we will look at the output from the XOR training with greedy random training.

Iteration #999996, Score=0.013418
Iteration #999997, Score=0.013418
Iteration #999998, Score=0.013418
Iteration #999998, Score=0.013418

Iteration #999999, Score=0.01341
Iteration #1000000, Score=0.01341
Final score: 0.013418057671024912

```
[1.0, 0.0]
> [0.9067663351025073], Ideal:
                                [:
[0.0, 1.0]
> [0.8703332321473845], Ideal: [1
[1.0, 1.0]
> [0.0064115711694006094], Ideal
    Of course, many individual
iterations were skipped. It also took a
sizeable number of iterations just to get
the score down to 0.01. You can see
from the above output that the actual
output does not exactly match the idea.
For the first input of [0,0], we can see
that the output should have been [0];
```

however, it was -0.16, which is fairly close. The two outputs that should have been [1.0] are both near 1.0, at 0.906

[0.0, 0.0] -> [-0.16770550224628078], Ideal: [0.0

and 0.87.

Training to the iris data set provides the following output:

Score=0.0874742 Iteration #99971, Score=0.0874742 Iteration #99972, #99973, Score=0.0874742 Iteration Score=0.0874742 #99974, Iteration Iteration #99975, Score=0.0874742 Iteration #99976, Score=0.0874742 #99977, Score=0.0874742 Iteration #99978, Score=0.0874742 Iteration #99979, Score=0.0874742 Iteration Iteration #99980, Score=0.0874742 Iteration #99981, Score=0.0874742 #99982, Score=0.0874742 Iteration

#99983, Score=0.0874742 Iteration #99984, Score=0.0874742 Iteration Iteration #99985, Score=0.0874742 Score=0.0874742 Iteration #99986, #99987, Score=0.0874742 Iteration #99988, Score=0.0874742 Iteration

#99989, Score=0.0874742 Iteration #99990, Score=0.0874742 Iteration #99991, Score=0.0874742 Iteration #99992, Iteration Score=0.0874742 Iteration #99993, Score=0.0874742 Iteration #99994, Score=0.0874742 Score=0.0874742 Iteration #99995, Iteration #99996, Score=0.0874742 Score=0.0874742 Iteration #99997, #99998, Score=0.0874742 Iteration #99999, Score=0.0874742 Iteration Iteration #100000. Score=0.08747

The above shows that the training continued until the score reached 0.08. This allowed the majority of the irises to be correctly classified, and was the result of using greedy random training and a very large number of iterations. In

the next chapter, we will get even better

0.08747428121794937

Final score:

results in fewer iterations using more advanced training algorithms.

Chapter Summary

This chapter introduced you to the fundamentals of training machine learning algorithms. Once trained, the machine learning algorithm should be able to produce output close to what you would expect from the input. When input is provided with the expected output, the algorithm has been provided with a training set. Training sets are used to train the algorithms.

Most machine learning algorithms keep a long-term memory, which is adjusted when the algorithm is trained. This long-term memory is often referred to as a weight or coefficient, and is typically stored in a vector.

This chapter described the greedy random training algorithm. The greedy

random training algorithm is a very simple training algorithm that assigns random values to long-term memory. New configurations are tried repeatedly

and the best configuration is kept. This is a very simple training algorithm that is often used as a baseline against which one might benchmark other algorithms. We trained two different models in

this chapter: a simple polynomial and an RBF model. The polynomial demonstrated how the greedy random algorithm can be applied to very simple equations. We were able to approximate the three coefficients used in the

polynomial.

The RBF model is based on radial basis functions, which are symmetric

basis functions, which are symmetric about a center. The RBF each have multi-dimensional centers and adjustable width values, although the width of an RBF is consistent across all dimensions. In this chapter, we used a Gaussian RBF.

The RBF model can be used for

The next chapter will introduce

classification or regression and uses training algorithms to modify its longterm memory. The long-term memory for the RBF model is made up coefficients, RBF widths, and RBF centers. The RBF model was used to learn the iris data set. These algorithms can be used to adjust the long-term memory vector used by the RBF network. They can be used on any algorithm that stores its state in a long-

additional optimization algorithms.

algorithm that stores its state in a longterm memory-like vector. The next chapter will describe hill climbing, simulated annealing and Nelder Mead training algorithms.

Chapter Optimization Training

- Hill Climbing
- Simulated Annealing
- Nelder Mead

This chapter will refine the concept of training a machine learning algorithm to provide more comiteplex approaches than those described in the previous chapter. There are many different algorithms for training machine learning algorithms. The algorithms presented in insight into the long-term memory vector they are attempting to optimize. This makes them very versatile in terms of what they can train.

This chapter will focus on

this chapter do not require any specific

optimizing continuous vectors, which are those that are made up of floating point numbers. Chapter 9 will focus on discrete problems.

Hill Climbing Training

Hill climbing is only marginally more complex to implement than the greedy random algorithm. One of the main disadvantages of the greedy random algorithm is that there is no refinement. A random vector is chosen for the long term memory and then immediately replaced if a better random vector is found. It does not attempt to refine a potentially good solution, but looks for a better one at random.

Hill climbing works by refining the

current vector, which is why the name is actually very descriptive of the algorithm. Imagine that you are randomly placed somewhere in the middle of hilly terrain and your goal is to climb to the highest location possible. You begin by looking at every location that you could reach in one step and then decide what step you are going to take. You always decide to take the step that moves you

until you cannot find a higher step. Once you cannot find a higher step, the process terminates. With hill climbing, the process terminates at the nearest high point, which is often called a local maxima.

the highest. This process is repeated

This process can also be run in reverse, if you seek to minimize. Instead of selecting the step that leads you to the highest possible position, you would select the step that leads you to the lowest position. The lowest position is called the local minima. Local minima

of training.

Using this same analogy, consider if you started out somewhere on the East

and maxima are very important elements

the Appalachian mountains, as walking to higher ground when starting on the East Coast would lead you to these peaks, and once you reached the peaks there would be no way to step higher.

However, they are not the highest ground in the world, or even in the United

States.

Coast of the United States and used hill climbing to find the highest place. You would probably get stuck somewhere in

This example presumes you are walking in a two dimensional space on the Earth's surface. The third dimension, or altitude, does not count because you cannot directly change your altitude. You

cannot fly! Yet, altitude is the objective. Altitude changes based your movements in the x and y dimensions. Most machine learning applications will have much more than two dimensions. However, the principle is still the same—these applications just have more dimensions to search.

You will very likely never find a global maximum or minimum for anything but a very trivial algorithm. Rather, you should hope to find successively better local minima or maxima. If you find your training to be "stuck," you will sometimes have to randomize and start over. You were probably stuck in a local minima or maxima (that is, stuck in Appalachians, instead of reaching the Himalayas). Hill climbing is greedy. Hill climbing would be unwilling to give up its spot on top of the Appalachians to ever find anything else.

The hill climbing algorithm is

implemented in two separate functions.

The first function performs an initialization for the hill climbing algorithm, while the second function shows an iteration. We begin with Listing 8.1, which shows one iteration of

the hill climbing algorithm. (Russell,

Listing 8.1: Hill Climbing Algorithm (Initialization)

2009)

```
function initHillClimb(
  ltm, // the initial long term me
  acceleration, // the acceleration
```

```
for i from 0 to ltm.length
   stepSize[i] = initialVelocity,
 candidate[0] = -acceleration;
      candidate[1]
1 / acceleration;
 candidate[2] = 0;
 candidate[3] = 1 / acceleration
 candidate[4] = acceleration;
    There are several different
implementations of the hill climbing
algorithm; this implementation makes
use of step size and acceleration. The
```

algorithm assumes that it will accelerate when it is moving in a direction that is

initial Velocity // the initial :

Listing 7.3 sets up two vectors for the algorithm to use. The **stepSize** vector tracks how big a step the algorithm is able to move in each

dimension. The parameter for this is defined by the term initialVelocity. The candidate vector defines five potential moves that the algorithm might take. The algorithm applies these candidate moves to each dimension. These potential moves are based on the acceleration parameter. The acceleration and initialVelocity parameters will affect the efficiency of your training. You will have to experiment with them in order to gain the best results.

Now that the algorithm has been initialized, we can begin processing iterations. Listing 8.2 shows the iteration function of the hill climbing algorithm.

Listing 8.2: Hill Climbing Algorithm Iteration

```
function iterateHillClimb(ltm)
 len = ltm.length;
// loop over all dimensions and t
 for i from 0 to len
  best = -1;
// We are trying to minimize, so
// Everything is lower than that
// score considered.
bestScore = +Infinity;
// Try each of the candidate move
   for j from 0 to candidate.lend
```

```
// Try the move and score, but ba
     ltm[i] = ltm[i] + (stepSize)
     temp = score.calculateScore
     ltm[i] = ltm[i] - (stepSize
// Keep track of what dimension
// improvement.
     if ( temp < bestScore)</pre>
       bestScore = temp;
       best = i;
// Now that we are done with the
// any other step produced a bett
// in that direction.
   if (best !=-1)
     ltm[i] = ltm[i] + (stepSize)
     stepSize[i] = stepSize[i] *
```

in a move. Once no further movement is possible, the algorithm has reached the local minima. The above function is designed to minimize the score function.

Adapting it to minimize is relatively simple. The examples provided for this example on GitHub support both minimization and maximization.

Hill climbing will typically perform better than the greedy random algorithm. However, like the greedy random algorithm, hill climbing is still typically used as a benchmark algorithm.

shown here optimizes continuous data, which has an infinite number of values between any two values. A different algorithm is used for optimization of discrete values, which have a fixed count. For example, the number of cars in a parking lot is a discreet number there are no fractional cars. Chapter 9 will describe how to optimize for discrete values.

The hill climbing implementation

Simulated Annealing

Scott Kirkpatrick and several other researchers developed simulated annealing in the mid-1970s. It was originally developed to better optimize the design of integrated circuit (IC) chips by simulating the process of annealing.

Annealing is the metallurgical process of heating up a solid and then cooling it slowly until it crystallizes. The atoms of such materials have highenergy values at very high temperatures. This gives the atoms a great deal of freedom in their ability to restructure themselves. As the temperature is

called rapid quenching—many irregularities and defects will be seen in the crystal structure. Ideally, the temperature should be reduced slowly to allow a more consistent and stable crystal structure to form, which will increase the metal's durability.

reduced, the energy levels of the atoms decrease. If the cooling process is carried out too quickly—a situation

emulate the annealing process. It begins at a very high temperature, at which the long term memory values are allowed to assume a wide range of random values.

Simulated annealing seeks to

As the training progresses, the "temperature" is allowed to fall, thus restricting the degree to which the

leads the simulated annealing algorithm to a better solution, just as a metal achieves a better crystal structure through the annealing process. (Das, 2005)

memory are permitted to vary. This often

Simulated Annealing Applications

Given a specified number of inputs

for an arbitrary equation, simulated annealing can be used to determine what inputs will produce the minimum result for the equation. In the case of the traveling salesman, this equation is the calculation of the total distance the salesman must travel. It is the error

calculation or scoring function for a machine-learning algorithm.

When simulated annealing was first

introduced, the algorithm was very popular for integrated circuit (IC) chip design. Most IC chips are composed of many internal logic gates, which allow the chip to accomplish the tasks that it was designed to perform. Just as algebraic equations can often be simplified, so too can IC chip layouts.

Simulated annealing is often used to find an IC chip design that has fewer logic gates than the original. The result is a chip that generates less heat and runs faster. The long term memory vector of a machine learning algorithm provides an memory values are used for the algorithm until one is found that produces a sufficiently low return from the error function.

excellent vector to optimize. Different

Simulated Annealing Algorithm

The simulated annealing algorithm

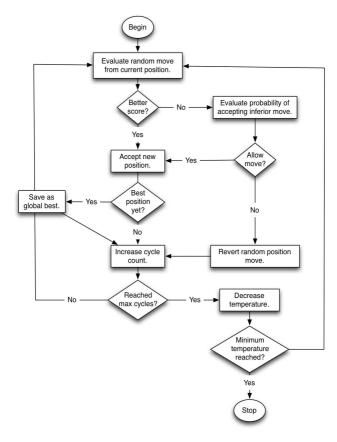
is similar to hill climbing in that it considers what moves it can make from its current position. These moves are evaluated randomly. If the randomly chosen move has a better score, than the current position, then the algorithm moves to the new position. If the new

position is a worse score, then the new

probability. This random probability is higher if the temperature is higher, as summarized in Figure 8.1.

position will be accepted with random

Figure 8.1: Simulated Annealing Flowchart



The ability to take on a worse score is an important distinction. Simulation annealing is not as greedy as the greedy random algorithm. Simulated annealing will sometimes take one step backwards to potentially take two steps forward.

The pseudo code to the complete algorithm is provided in Listing 8.3.

Listing 8.3: Simulated Annealing Pseudo Code

```
function iteration(
  ltm, // the long term memory we 
  cycles // the number of cycles p
)
{
  len = ltm.length;
  k++;
```

currentTemperature = coolingSche

```
for cycle from 0 to cycles
// backup current state
oldState = ltm.clone();
// randomize the method
  performRandomize(ltm);
// did we improve it? Only keep t
// if it improved (greedy).
      trialError = calculateScore
// was this iteration an improver
keep = false;
 if trialError < currentError
  keep = true;
else
 {
   p = calcProbability(
         currentError,
         trialError,
         currentTemperature);
   if (p > rand())
```

```
// should we keep this new posit:
 if (keep)
   currentError = trialError;
 // better than global error
   if (trialError < globalBestEr:</pre>
     globalBestError = trialErro:
     oldState = ltm.clone();
     globalBest = ltm.clone();
else
   ltm = oldState.clone();
 }
    The above code performs
```

keep = true;

obtaining the current temperature from the cooling schedule. This temperature will remain the same for the entire iteration. The iteration will execute a defined number of cycles. For each cycle, the algorithm will attempt to move from the current position. Each cycle will take place at the same temperature.

iteration of the simulated annealing algorithm. The iteration begins by

on the current position. Because of this, only close positions will be considered. If the new position has a better score than the current position, then the algorithm moves to the new position.

For each cycle, a random position

based on the previous error, the current error, and the current temperature. The exact process used to calculate the probability will be described later in this chapter.

At the end of the iteration, the

Otherwise, it calculates a probability

algorithm checks to see if it has surpassed any previous best solutions. In this regard, the algorithm is ultimately somewhat "greedy" in that it always keeps the best solution that it has found so far.

Cooling Schedule

The cooling schedule defines how quickly the temperature will fall during

the simulated annealing iterations. The temperature determines the likelihood that an algorithm will move to a new position with a worse score. It is best if this probability is higher in the beginning phases of the training. Once the training has run for a longer time, it is best if the probability of moving to a worse position is much less. This allows the algorithm to narrow in on a more optimal solution. The following equation is used to calculate the cooling schedule.

Equation 8.1: Cooling Schedule

$$T(k) = T_{init} \frac{T_{final}}{T_{init}}^{\frac{k}{k_{max}}}$$

The above equation calculates the

temperature for iteration number k. There are a few things to keep in mind when setting the equation.

with the initial and final temperatures, as well as the max number of iterations.

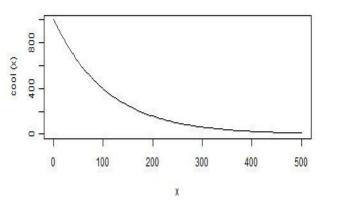
The equation must also be provided

- It is not necessary that you use this equation exactly.
- It is important that the temperature decrease as training progresses.
- Do not choose zero as the final temperature in the above equation. It is okay to choose something close to zero, however. Because the above equation multiplies by the

final temperature, having a final temperature of zero will quickly take the current temperature to zero.

You can see this cooling schedule in Figure 8.2.

Figure 8.2: Cooling from 1,000 to 10.500 Iterations



The temperature is used to determine the probability that the algorithm will accept an inferior score.

Annealing Probability

good a score as the previous location. A completely greedy algorithm would never consider a new position that produces a worse score. However, such an outlook can be counterproductive. You might have to go through a few valleys before you find the top of the highest mountain!

Simulated annealing always

attempts to move the algorithm to random locations. Sometimes these random locations will not produce as

We will compute the probability that the simulated annealing algorithm will accept a worse score as a function of the following three inputs:

- Current error
- Previous error
- Current temperature

Equation 8.2 makes use of all of these.

Equation 8.2: Annealing Probability

$$P(e, e', T) = \exp(-(e' - e)/T)$$

The probability function accepts the previous error, current error, and current temperature. The probability function returns a number between 0 and 1. A value of one means a 100% likelihood of selecting a worse score, and a value of zero means there is no likelihood of selecting a worse score. These numbers

numbers. If the random number is less than the probability, then we will accept the solution with an inferior score. Equation 8.2 returns higher

can easily be compared against random

probabilities for higher temperatures. However, the increase in error is also considered. The larger the increase in error, the new position is less likely to be accepted.

Simulated annealing can also be used to train the RBF networks introduced in the last chapter. It allows for more efficient learning than could be achieved with the hill climbing and greedy random algorithms alone.

Nelder Mead

The Nelder Mead algorithm was proposed by John Nelder and Roger Mead (Nelder, 1965). It is an optimization algorithm that can be used to optimize vectors to a scoring function. The Nelder Mead method is sometimes called the downhill simplex method or amoeba method. Nelder Mead is relatively easy to visualize and understand. It is also a generally effective solutions finder. It thus provides a great introduction advanced training algorithms.

Nelder Mead works by constructing a simplex. A simplex is a geometric

to N+1, where N is the number of dimensions in the problem. A vertex is a point in space. These vertices become the corners of a geometric shape called a simplex. Lines are drawn to form new shapes that connect vertices, or corners.

shape that has a number of vertices equal

If we were optimizing a vector with two dimensions, we would have a simplex in the shape of a triangle.

The simplex is simply a list of

potential solutions. The algorithm always keeps N+1 potential solutions, and so the simplex will change its shape as training progresses. Once the training has reached an advanced state, the simplex has most become very small. At this point, we can find the solution by

selecting the vertex with the best score. The Nelder Mead algorithm can

also be used to train the RBF networks introduced in the last chapter. It is able to converge to a low error faster than greedy random, hill climbing, and often simulated annealing algorithms.

Nelder Mead always begins with an initial guess as to the solution vector. If you cannot make an educated guess, then choose a random vector. If you previously trained with another algorithm, you can use your result from the last algorithm as the initial guess, and Nelder Mead will further refine the solution. This also works if you want to

refine a previous Nelder Mead solution.

the vertices of the starting simplex. If we have two dimensions, then we need to generate two additional vertices. The simplex is always constructed of N+1 vertices, where N is the number of dimensions. It is important that you not confuse dimension with vertex. A vertex is a point made up of one or more

The initial solution becomes one of

We will now consider Nelder Mead for two dimensions. The following would be true in this case.

• Dimensions = N = 2

dimensions.

- Vertices = N+1 = 3 (a triangle)
- Simplex: A collection of 3 vertices,

each having 2 dimensions (resulting in the shape of a triangle)

The first step for Nelder Mead is to

generate the initial simplex. This simplex will be refined as the iterations

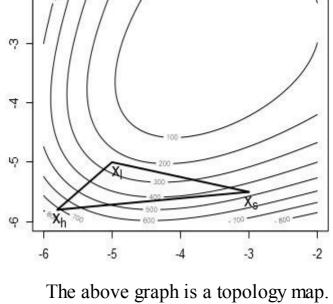
progress. The initial simplex always takes the initial solution vector as one of the starting vertices. The other N vertices are created by moving one of the N dimensions by a set amount. Typically, the sides of the initial simplex are set to be of the same length.

Figure 8.3 shows a visualization of

a three vertex simplex in two

Figure 8.3: Nelder Mead Simplex

dimensions.



I sometimes like to think of the vertices in the above figure as members of a search party covering rugged terrain. All are looking for the optimal point on the

or a low, depending on how you define a good score. In a nutshell, Nelder Mead works by moving the searcher who is in the worst position to a new location that is based on the better positions of the other two.

map. The optimal point might be a high

The minimum that the depicted simplex is moving toward is in the large oval-like area in the top-right. The vertices are labeled **X**, although they are not to be confused with x and y dimensions. The three **X** vertices are labeled **h**, **s**, and **l**. They are the worst, second worst, and the best vertices, respectively.

Iterations of Nelder Mead consist

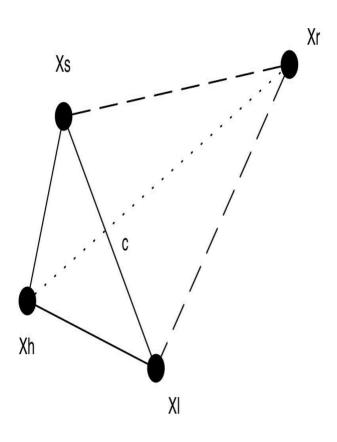
of the following steps:

- Step 1. Find the worst, second worst, and best points of the vertex.
- Step 2. Reflect the worst to a better point through the best side.
- Step 3. If the reflection is successful, expand.
- Step 4. If the reflection it unsuccessful, contract.

Reflection

Reflection is the first step in the Nelder Mead algorithm. The worst vertex will be the one considering a move. Figure 8.4 shows the basic setup for moving by reflection.

Figure 8.4: Reflection



the solid lines, and the worst position is Xh. To reflect Xh, the average is taken between Xs and Xl. This gives a center, which is labeled as c in the figure above. If you consider the search party example, the farthest off searcher (Xh) looks in the direction of the other two and points at the center point (the average) between them as the best place to go. Because the other two are in better locations than him, the searcher must assume that anything behind him is also worse. He must move toward the other two, so he visualizes a point well beyond them, at point Xr. He visualizes a point well beyond because he aspires to become the best searcher!

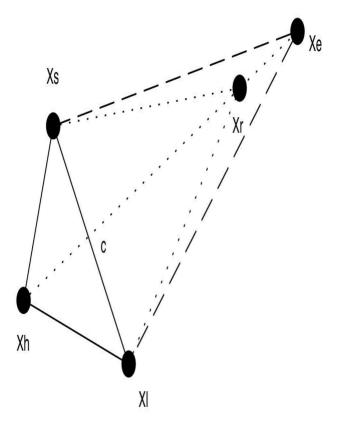
The current simplex is depicted by

After selecting the point at Xr, the point is now evaluated. Was it actually a better location? If it was, then we continue by implementing expansion. If not, then we continue by implementing contraction.

Expansion

Continuing the example from before, the Xh searcher has seen that he could improve his ranking by moving to Xr. Now he gets a little greedy, and wants to move farther. If we are climbing down a valley, then going to a farther point will probably get us to the optimal point faster. Figure 8.5 depicts this scenario.

Figure 8.5: Expansion



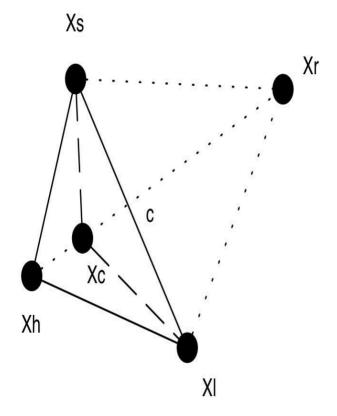
The searcher at Xh evaluated the spot at Xr. It was an improvement. So he became greedy and jumped right to Xe without checking Xe. This is okay, since even if he overshoots, he was at the worst spot to begin with.

This ends the iteration. The next iteration re-evaluates all of the vertices and determines which is now the farthest off.

Contraction

Contraction occurs when the reflection point does not improve the rank of the worst point. Figure 8.6 shows the contraction scenario.

Figure 8.6: Contraction



Continuing with the searcher analogy, the worst searcher at Xh had dreams of moving to Xr and getting a better rank. However, if the position at Xr had an even worse score, all we can do is move closer to the other two searchers. We still point toward the center of the two other searchers but, since our hopes have been dashed, we do not move beyond them. We move somewhere in the middle of the simplex, to location Xc. Hopefully this improves our rank. Either way, the iteration is now done. The next iteration will rank the vertices again and continue.

Finishing the Nelder Mead Algorithm

It is important to know when to terminate an iterative algorithm such as Nelder Mead. This algorithm typically terminates based on the following three criteria.

- A maximum number of iterations is exceeded.
- The score is good enough.
- The vertices have become "close enough" to each other.

Once the algorithm completes, we consider the best vertex to be the

simplex based on the best vertex. The search can then begin anew.

Nelder Mead is relatively efficient in that only one of the vertices needs to be reevaluated with each iteration. In

solution. If the vertices have become close together, another option is to restart the algorithm by building a new

machine learning, most computer processing time is spent evaluating against the training data. With Nelder Mead, it is only necessary to reevaluate one vertex because only the worst vertex moves.

In addition to reflection,

In addition to reflection, contraction and expansion, some older implementations of Nelder Mead also made use of a shrink step. Later research

however, and most modern implementations of Nelder Mead do not include it.

Unlike greedy random, simulated

found the shrink step to be unnecessary,

annealing and hill climbing, Nelder Mead performs a coordinated search from multiple locations at once. Such coordinated searches are very common in even more advanced algorithms. Particle Swarm Optimization (PSO) and Genetic Algorithms both use many multiple coordinated solutions.

Chapter Summary

This chapter introduced you to three optimization algorithms that can be used for training. These algorithms are designed to optimize individual values in a vector to obtain a better score for the model being trained. This vector is the long term memory for any of the machine learning algorithms we have seen so far.

Hill climbing is a simple search optimization algorithm. It starts at a vector location and evaluates moves that can be made from that vector. Whatever move results in the largest improvement to the score is taken. Hill climbing is

maxima. Once hill climbing reaches a point where it can no longer find a better solution, the algorithm is complete.

Simulated annealing works

very susceptible to local minima and

somewhat like hill climbing, except that simulated annealing is sometimes willing to move to a position that has a lower score than the current position. Nelder Mead is another training

algorithm that can be used to optimize a vector.

This chapter focused on continuous optimization algorithms. A continuous optimization algorithm deals primarily

optimization algorithms. A continuous optimization algorithm deals primarily with floating point numbers. However, some optimization algorithms may be used on discrete data. The next chapter



Chapter 9: Discrete Optimization

- Discrete vs. Continuous
- The Knapsack Problem
- The Traveling Salesman Problem

In the last chapter, we saw that simulated annealing could be used to optimize the long-term memory of machine-learning algorithms. The optimization occurred against the long-term memory vector of a machine-learning algorithm. This vector was composed of continuous floating-point numbers. With continuous vectors, there

whole numbers. This is continuous data. Not all data is continuous.

This chapter will focus on using simulated annealing to analyze discrete problems, particularly focusing on the

is an infinite amount of additional numbers between two consecutive

traveling salesman problem and the knapsack problem. The traveling salesman problem is discrete because it seeks to find the most optimal route to visit a fixed number of cities. The knapsack problem is discrete because it seeks to find an optimal set of items to put into a finite knapsack. Discrete data always deals with a finite number of items.

The Traveling Salesman Problem

Simulated annealing is commonly used to solve the traveling salesman problem (TSP), because the TSP is an NP-hard problem that generally cannot be solved by traditional iterative algorithms. TSP is one of most famous computer science problems. We will now see how to apply simulated annealing to it.

Understanding the Traveling Salesman Problem

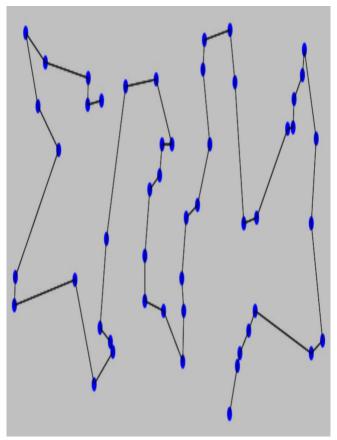
involves determining the shortest route for a "traveling salesman" who must visit a certain number of cities. The salesman is allowed to begin and end at any city, but must visit each city once and only once. There are several variants of the TSP, some of which allow multiple visitations to cities or assign different values to different cities. The TSP we will evaluate in this chapter simply seeks the shortest route to visit

The traveling salesman problem

shown in Figure 9.1.

Figure 9.1: The Traveling Salesman

each city once. The TSP problem and shortest route used in this chapter are



It may seem like finding the shortest route would be an easy task for a normal iterative program. However, as the number of cities increases, the number of possible combinations increases drastically. If there are one or two cities, only one route is possible. If there are three cities, the possible routes increase to six however. The follow list shows

to six, however. The follow list shows how quickly the number of paths grow!

1 city has 1 path
2 cities have 1 path
3 cities have 6 paths
4 cities have 24 paths
5 cities have 120 paths
6 cities have 720 paths
7 cities have 5,040 paths
8 cities have 40,320 paths

9 cities have 362,880 paths 10 cities have 3,628,800 paths

12 cities have 479,001,600 paths
13 cities have 6,227,020,800 path
...
50 cities have 3.041 * 10^64 path

The formula used to collect data for

11 cities have 39,916,800 paths

the above table is the factorial. The number of cities, n, is calculated using the factorial operator (!). The factorial of some arbitrary value n is given by n * (n-1) * (n-2) * ... * 3 * 2 * 1. These values become incredibly large when a program must do a "brute force" search. However, a simulated annealing algorithm such as the sample program examined in the next section finds the solution to a 50-city problem in a matter of minutes. (Behzad, 2002)

Implementing the Traveling Salesman Problem

So far, we have discussed the basic principles of continuous simulated annealing algorithms in previous chapters. The discrete version of simulated annealing is not too different from the continuous version that we saw in Chapter 8. The flow chart remains the same as what we saw in Figure 8.1. The difference is in how we move from the current position.

To conduct continuous simulated annealing, we would add a random value to one or more dimensions to move from the current position. In

creative. In the context of the TSP, each solution is a path through the cities. Our current position is this path. Moving to a new "position" means choosing a path similar to the current path.

discrete simulated annealing, on the other hand, we need to be a little more

It is important not to confuse the term "position" with city location. In this context, it does not refer to any particular "position" within the map of the cities. Rather, it describes one path among all possible paths to navigate that particular map. To move from one path

the cities. Rather, it describes one path among all possible paths to navigate that particular map. To move from one path to another, we simply flip the order of two cities in the original path. Flipping two cities ensures that we do not introduce a duplicate city.

solution. For TSP, this is a random list of the cities, with no duplicates. Then you must provide a means of creating a new solution through the implementation of a slight, randomized change For TSP, we simply flip the order in which the path visits two cities. This is implemented by choosing two random indexes (that are not the same) and exchanging their locations on the list.

To use simulated annealing, you

must first generate an initial random

There are three things that you must provide to any simulated annealing algorithm implementation.

• A scoring function to evaluate each

- position.
- A means of generating an initial random potential solution.
- A means of moving to a new random position based on your current position.

This is no different from continuous

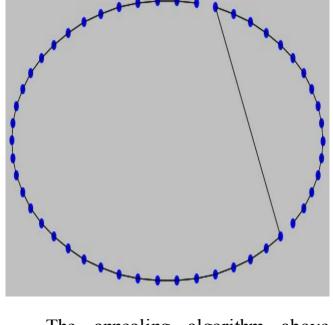
simulated annealing. The primary difference between the continuous and discrete annealing is in how these three aspects are implemented. For the traveling salesman problem, the score is simply the distance traveled, which is scored more highly as the distance travelled minimizes. The initial solution is the generation of a random, nonrepeating list of cities. Movement to the



Circular TSP

How can we evaluate an algorithms effectiveness with an NP-Hard problem? For an NP-Hard problem we often do not know the actual correct answer. This can make it very difficult to know exactly how close the algorithm has come to an optimal solution. There is a way to test the simulated annealing algorithm on a TSP, however. We can arrange the cities in a circle. If the cities are arranged in a circle, or oval, then the optimal path should run the perimeter of the shape. Figure 9.2 shows simulated annealing trying to optimize a path through cities arranged in an oval.

Figure 9.2: Annealing an Oval Path



The annealing algorithm above came close to an optimal solution. However, it is not perfect. This is okay.

insight into geometry that we can immediately spot that this path is not perfect. If you have insight into a problem that can help to solve it, then by all means, use it! AI is most useful when you have no other way to solve a problem.

You can rarely find a global optimum in any situation. It is only because we have

The Knapsack Problem

combinational optimization problem that has been around as early as the late 1800s. The origin of the name is unknown, although mathematician Tobias Dantzig suggested that the knapsack problem may have originated as a folk story long before a formal

The knapsack problem is a

Understanding the Knapsack Problem

mathematical problem was set down.

The knapsack problem describes the dilemma of a burglar inside of a store. He is surrounded by merchandise, should the burglar take to maximize his profit? The combination of items must fit inside his knapsack.

In fact, anyone who has packed for

but he only has one knapsack. What

a trip has faced a variant of the knapsack problem. Figure 9.3 shows a knapsack and some items one might want for an overnight camping trip.

Figure 9.3: The Knapsack Problem



The knapsack problem is a discrete problem. You can only select a fixed number of items and you are typically allowed to choose only zero or one of each item. This is the most common type of knapsack problem and it is called a 0-1 problem. Other variants allow for the selection of more than one of each individual item. The items are typically provided to the problem with weights and profit scores. You might wonder about volume in the knapsack problem. By convention, the knapsack problem

By convention, the knapsack problem does not consider volume. The maximum weight that will fit in the knapsack is also specified. (Pisinger, 2003)

Implementing the Knapsack

Problem

Discrete simulated annealing can easily be applied to the knapsack problem. It is very important to think about how you might want to represent this problem. In the context of the knapsack problem, a solution is a list of items that does not exceed the weight limit imposed by the knapsack.

The best way to represent a potential knapsack solution is with a vector that has dimensions equal to the number of unique items that can be added to the knapsack. Each item's element in this vector will contain a whole number representing the count of

that item taken. For example, Figure 9.3 describes the potential for bringing the following items.

Coffee thermos (weight=5,profit=1)
Baseball cap (weight=1, profit=1)
Blanket (weight=3, profit=10): table to be water (weight=2, profit=1)

Out knapsack can hold a max

weight of 7. The coffee thermos has been deemed unworthy, so that value is **false**. The rest has been determined to be profitable, so their values are **true**. The resulting weight is 6, which is below the maximum weight of 7. Adding the coffee would put us over the weight, while replacing anything else with the coffee would reduce our profit.

the solution. We must provide certain things to the simulated annealing algorithm.

We now have a way to represent

position (set of items).A means of generating an initial random potential solution.

A scoring function to evaluate each

 A means of moving to a new random position based on the current position.

Simulated annealing always solves a minimization problem. This aspect must be considered during the creation of the scoring function. We would like to

tie the maximum score to the profit

generated by each item we take. The theoretical maximum profit is the sum of the profit of all items. If all the items fit in the knapsack, the theoretical maximum profit is attainable—otherwise, it is not.

We will use the difference between

our current profit and the theoretical maximum as the best score. It is unlikely that we will ever get the optimal score of zero, which would indicate that every item can fit in the knapsack. If they can all fit, it hardly seems worthwhile to consider the problem. Rather, we

instead attempt to approach perfection.

Another important feature to consider for the scoring function is what happens if the knapsack's maximum weight is exceeded in the solution.

hurt to check the maximum weight in the scoring function as well. If the knapsack's maximum weight is exceeded, then the score should be pushed out to a very large value. This will cause any invalid knapsack

Ideally, our randomization would never let this happen. However, it does not

configuration to be discarded by the algorithm.

To meet the second provision to simulated annealing, we need a way to initialize a random solution. To initialize the first solution, start with an empty knapsack and add items to it one at a

time. Once we add an item that exceeds the maximum weight of the knapsack, remove that item and consider the To meet the third provision to simulated annealing, we need to generate

knapsack initialized.

a new position based on the current position. To randomize to a new state, add a new item that is not already in the knapsack. If this sets us over the maximum weight, choose a random item and remove it. Continue to remove items until the knapsack is below the maximum weight. The result will be the new position.

Chapter Summary

This chapter looked at how we might apply simulated annealing to a discrete problem. Discrete solutions are usually members of a finite set. For example, whole numbers in a range are discreet, as are colors.

There are very few differences between a continuous simulated annealing algorithm and a discrete one. Both require three components:

- A scoring function.
- A way to generate an initial random solution.

 A means of slightly changing a solution as we iterate through potential solutions.

The traveling salesman problem

was introduced as a discrete problem. The traveling salesman seeks the shortest possible path through a number of cities. Brute force cannot be applied to this problem, as there are too many possibilities. Simulating annealing can be used to find an acceptable solution, however. The end result from simulated annealing may not be the global optimum, however, as finding the best solution is typically NP-Hard.

The knapsack problem is also discrete. This problem requires you to

varying weights and profit values to pack into a knapsack that can only hold so much weight. The goal is to maximize the profit for the weight our knapsack can hold.

The next chapter will conclude this

choose from a list of items that have

book by introducing linear regression and general linear models. These are two very common statistical models that can be used with machine learning. Both linear regression and general linear models are valuable when used alone or as part of a larger algorithm.

Chapter 10: Linear Regression

- Linear Regression
- Generalized Linear Model (GLM)
- Link Function

This chapter will explore linear regression and generalized linear models (GLM). These are related statistical models that allow relationships to be established between input and output vectors. The input vector can contain multiple values, while the output vector must be a single value.

linear relationships to be modeled between the input and output vectors. These relationships can be used for

Linear regression allows for simple

some to learn basic problems, so long as the relationships are linear. Generalized linear models (GLM) add a link function to regular regression that greatly expands what can be modeled, as the relationship no longer needs to be linear.

(Pedhazur, 1982)

Linear Regression

Linear regression attempts to map the input vector to the output vector with a relatively simple linear model. If you just have two variables, **x** and **y**, you can write a linear function from them. Equation 10.1 shows such an equation.

1

Equation 10.1: Linear Function

Y = mx + b

Here **m** is the slope and **b** is the x-intercept. This function is called linear because on a graph it looks like a straight line. A curve in the line would indicate that the function is not linear.

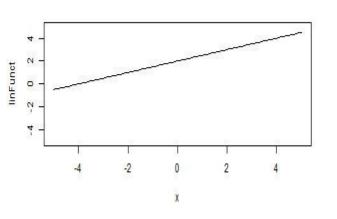
The following equation gives

values to the unknowns in Equation 10.1. Y = 0.5x + 2

$$I = 0.01 + I$$

The slope is 0.5 and the x-intercept is 2. Figure 10.1 shows the graph of this equation.

Figure 10.1: Graph of Y = 0.5x + 2



variable linear regression model. A linear regression dealing with only a single variable is called univariate. A very common example used to demonstrate univariate regressions is the relationship of shoe size to a person's height. This regression would accept a single input of the person's height and output their shoe size, or vice versa. Training such a model would involve finding the slope and y-intercept that describes the relationship between height and shoe size.

Equation 10.1 is a simple, single

The above graph shows that the function is linear. The function has a positive slope, which is evident in the line's northeast to southwest orientation.

not greatly inclined. Because the yintercept is 2, we know that when x is zero, y will be 2.

Many problems consist of several

inputs, however. Such models are called multivariate. A multivariate linear regression looks very similar to a

The slope is also only 0.5, so the line is

univariate. The only difference is that you have one term for each of the inputs. Additionally, you still have the y-intercept. Equation 10.2 shows the general form of a multivariate linear regression.

Equation 10.2: Multivariate Linear Regression

 $y_i = \beta_1 x_{i1} + \dots + \beta_p x_{ip} + \varepsilon_i = \mathbf{x}_i^{\mathrm{T}} \boldsymbol{\beta} + \varepsilon_i, \quad i = 1, \dots, n$ In the above equation, the **x**

variables represent the input vector. There will be a total of \mathbf{n} inputs. You should notice that each of the inputs is

multiplied by a corresponding beta value. Finally, an epsilon value is added. Epsilon represents the y-

intercept. Despite all the additional terms, the above equation is still linear. Any such model would produce a straight line graph.

We will focus on the multivariate

We will focus on the multivariate linear regression. Univariate linear regression is really just a special case of multivariate regression. Thus, it is not worth learning to do two separate algorithms.

coefficients. Even epsilon is a coefficient of one. These coefficients make up the long-term memory for this model. We could use any of the learning algorithms presented in this book to find decent coefficients that produce the desired outputs from the inputs in your training set.

The beta and epsilon values are

Least Squares Fitting

determining what coefficients will most closely match your training set. Once you have your coefficients, it is easy to calculate the output of a linear regression. It is unlikely that coefficients

Training is the process of

will be fit enough to allow the model to represent every training case. However, training will attempt to minimize the overall error of your training set elements.

Most documentation on linear

regression uses the word "fitting"to describe the process of training. Both terms really mean the same thing. As stated in the previous section, you could use any of the training algorithms in this book to fit proper coefficients to the model. The training algorithms presented are all general-purpose algorithms. They do not specify any requirements on the long-term memory (in this case, coefficients) that they are

trying to fit. We will now see a training algorithm designed specifically for linear regression.

Often, mathematical solutions will

produce a better solution faster than

general algorithms. If you do not know of an appropriate mathematical solution, then by all means use a general algorithm. The only real downside is that the training time will likely be longer. I've occasionally implemented a general solution only to have a more mathematically advanced friend say, "Oh interesting, you decided not to go with the [insert advanced mathematical technique here] approach." Though, I am always quite glad to have such shortcuts shown to me. Math is an infinite loop of Now we will look at one such mathematical solution in order to use

learning.

least squares fitting. This training algorithm will not work on any of the previous models or machine learning algorithms presented in this book. The only algorithm in this book with which you can use least squares fitting is linear regression, as least square fitting is not a general-purpose algorithm.

create two matrixes. These matrixes will be named **matrixX** and **matrixY**. Both matrixes will have a number of rows equal to the number of training set elements. The matrix **matrixX** will hold

To fit using least squares, we must

equal to the input count plus 1. Each input in the matrix should have a one concatenated to it. This allows the y-intercept to be accounted for. The matrix

matrixY will hold all of the ideal outputs from the training set. For linear

all of the inputs from the training set. Thus, it will have a number of columns

regression, there should be only one output, so the column count for **matrixY** will always be 1.

Using these two matrixes, we can get a good fit of coefficients for the

get a good fit of coefficients for the linear regression. We will use a linear algebra technique called matrix decomposition, of which there are many different kinds. Matrix decomposition is essentially a factorization. Factoring the

matrix separates the matrix into two matrixes that, when multiplied together, produce the original matrix.

For sum of squares, we will not use the two factor matrixes, but rather use the QR decomposition to solve this system of equations. QR decomposition is commonly used in AI. It is the main component of the least squares training algorithm. (Barlow, 1993)

Least Squares Fitting Example

Let's create a linear regression model that will convert Fahrenheit temperatures into Celsius using least squares fitting. We will begin with some training data.

0 -> 32 100 -> 212

The above data simply states that 0 degrees Celsius is equal to 32 degrees Fahrenheit. Likewise, 100 degrees Celsius is 212 degrees Fahrenheit. We would like to calculate the slope and y-intercept for a linear equation that will produce the desired output shown above.

We must generate the **matrixX** and **matrixY** matrixes. First, we generate **matrixX**. As previously stated, this is essentially the input values with a 1 concatenated. The 1 represents the y-

[0.0,1.0]

intercept. **matrixX** is described below.

Next, we construct **matrixY**, which is a matrix of ideal outputs.

[32.0]
[212.0]

The next step is to solve the matrix,

[100.0,1.0]

coefficients. I am not going to show you the internals of a QR decomposition, as this is a "wheel" I've never tried to reinvent. I always use a linear algebra package to perform this operation. There are quite a few linear algebra packages to choose from in most programming

using QR decomposition, and obtain the

GPU based linear algebra package. BLAS is a very common linear algebra package, and there is a version of BLAS for CUDA GPUs called CUBLAS. GPUs can often perform matrix operations considerably faster than CPUs.

We will solve matrixX for

languages. Some are very efficient. You might choose to use a natively implemented linear algebra package or

matrixY using QR. This will return the coefficients that must be applied to matrixX to produce matrixY. We will only get one set of coefficients, despite the fact that we have two rows. These coefficients will produce the best results possible over all rows. This results in the following matrix:

```
[1.8]
[32.0]
```

The matrix describes a coefficient and the y-intercept. The y-intercept is always given by the one that we concatenated to every input. As previously stated, the y-intercept has a coefficient of 1. Therefore, the following linear model can be used to convert Celsius to Fahrenheit:

```
f = (c*1.8) + 32
```

This matches the conversion formulas found in Wikipedia and other sources.

There are no iterations with the least squares fit. It is not necessary to

perform multiple iterations of least squares fitting, unlike other iteration-based algorithms seen in previous chapters.

Anscombe's Quartet

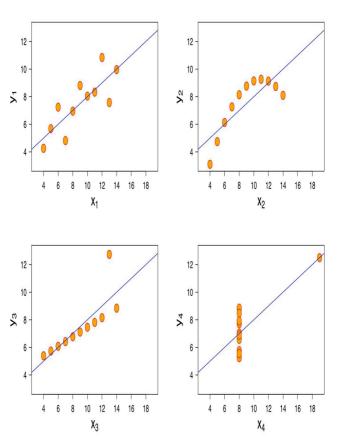
Anscombe's Quartet

Linear regression requires that the relationship between inputs and outputs be linear, but it can be problematic to force a line from data points. Anscombe's Quartet is a special data set

that points out some issues in linear

regression. Figure 10.2 shows Anscombe's Quartet. (Anscombe, 1973)

Figure 10.2: Anscombe's Quartet



of these produce the exact same linear regression coefficients. The line drawn through the points represents the linear regression. That these four all produce the same linear regression indicates some of the flaws in the system. The top-left plot shows a linear regression line that does a pretty good job approximating the relationship between the points. However, the topright data set is not at all linear. The

bottom two show the effect that outliers can have on a model. An outlier occurs when a small number of points are completely out of sequence with the

The above figure shows four

different data sets. The points in each of these four look clearly different. All four others.

Abalone Data Set

An example is provided for fitting a linear regression to the Abalone Data Set, which contains observations of abalone sea snails. The data set can be obtained from the following URL.

http://archive.ics.uci.edu/ml/datasets/Aba

The set fits a linear regression to predict the number of rings in the abalone using a number of other observations. Much like a tree, the ring count of an abalone indicates its age. The output from this set is as follows. (Nash, 1994)

```
> [7.75634765625], Ideal: [7.0]
[1.0, 0.0, 0.0, 0.53, 0.42, 0.13!
> [11.078125], Ideal: [9.0]
[0.0, 1.0, 0.0, 0.44, 0.365, 0.12]
> [9.5615234375], Ideal: [10.0]
[0.0, 0.0, 1.0, 0.33, 0.255, 0.0]
> [6.69970703125], Ideal: [7.0]
[0.0, 0.0, 1.0, 0.425, 0.3, 0.09!]
> [7.7802734375], Ideal: [8.0]
[1.0, 0.0, 0.0, 0.53, 0.415, 0.1!
> [13.52197265625], Ideal: [20.0]
```

[0.0, 1.0, 0.0, 0.455, 0.365, 0.0] > [9.1279296875], Ideal: [15.0] [0.0, 1.0, 0.0, 0.35, 0.265, 0.0]

It provides the ring count predicted for each abalone, as well as the ideal ring count according to the training data.

Generalized Linear Models

Generalized linear models (GLM) are based on the linear regression models discussed above. They make use of a link function to further abstract the output from the GLM. There are a variety of link functions that can be used with GLMs. Because GLMs are trained with a calculus-based training algorithm, the link function must have a derivative. The use of derivatives for GLM training will be described in the next section.

The equation for a GLM is very similar to that for linear regression. The primary difference is that a GLM adds a link function.

The equation for a GLM is shown in Equation 10.3.

Equation 10.3: Generalized Linear Model

$$y_i = g(\beta_1 x_{i1} + \dots + \beta_p x_{ip} + \varepsilon_i = \mathbf{x}_i^T \boldsymbol{\beta} + \varepsilon_i), \quad i = 1, \dots, n$$

You may have noticed that Equation 10.3 is very similar to Equation 10.2. This is because the GLM is essentially the return value of a linear regression passed to the link function. In the above equation, the link function is given by g(). The input vector is x, while the output is v. The beta values make up the coefficients and the epsilon value is the y-intercept, which is the same as with linear regression. The only addition is

There are many different link functions to choose from. One of the most common is the logistic, or logit,

the link function.

function. A GLM that uses the logit function is typically called a logistic regression model. The output of a logistic regression is always considered to be one of two values.

If you would like to model

to be one of two values.

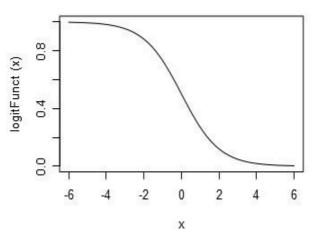
If you would like to model something with two categories, then you should consider using a logistic regression model. Logistic regression chooses between two options based on

chooses between two options based on the input. This might be true/false, good/bad, buy/sell, etc. If you need to choose between more than two options, you could use the RBF networks The logit function is sometimes called a sigmoid function. It is shown in

presented in this book.

called a sigmoid function. It is shown in Figure 10.3.

Figure 10.3: The Logistic Function



The logistic function is able to scale the output from the linear regression. It has several very important properties:

- g(-Infinity) = 0g(Infinity) = 1
- g(0) = 1/2• g(-x) = 1 - g(x)
- if x > y then g(x) > g(y)

The output of the logit will never be less than zero or more than one. Therefore, 0 is typically mapped to one of the categories that the GLM aims to predict, while 1 is mapped to the other category. A value of 0 results in a half,

The sigmoid function is also monotonic. Monotonic refers to the fact that the function is either consistently increasing or decreasing. Monotonic functions do not reverse that direction.

which is exactly between 0 and 1.

Reweight Least Squares Training GLMs can be trained using any of

the general training algorithms presented in this book. However, there is a mathematical shortcut in the form of the reweight least squares training algorithm. This training algorithm is based on the least squares training, but reweight least squares training can handle the addition of the link function. Unlike least squares, the reweight least squares algorithm is iterative. You will need to process iterations until the error is acceptable. (Chartrand, 2008)

The reweight least squares

algorithms called gradient descent. The back propagation-training algorithm also falls under the category of gradient descent; you might be familiar with back propagation training if you've ever worked with neural networks.

algorithm falls into a category of training

Gradient descent makes use of calculus to determine the gradient of the error function at the current state of the long-term memory (the coefficients). This gradient will indicate whether we need to increase or decrease each coefficient to lower the error. To do this, we need to determine the derivative

need to increase or decrease each coefficient to lower the error. To do this, we need to determine the derivative of the link function, which means that link functions must be differentiable (have a derivative) in order to perform

The derivative of a function is just another function. The derivative function tells us the instantaneous rate of change for the first function. Consider a function

gradient descent.

that describes the position of a car at any given time. If you pass the value 10 seconds into the function, it tells you the position of the car at 10 seconds. Likewise, if you pass in 60 seconds, you

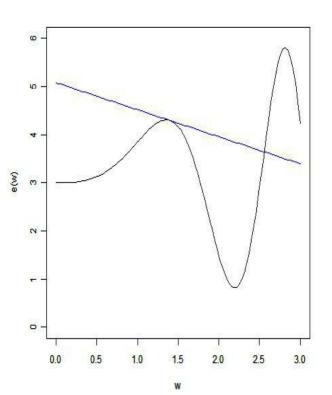
will be given the position of the car at that time. If you were to take the derivative of the function describing position at time, you would have a new function that describes the speed of the car at any time.

When plotted on a graph, the derivative usually looks like a line that

point. Consider whether Figure 10.4 represents the error as you varied only one coefficient.

touches the main function at only one

Figure 10.4: Error Derivative from Varying Single Coefficient



how the slope of the derivative tells us the direction in which the underlying function is heading. The goal is to descend to the lowest point, which is somewhere between 2.0 and 2.5. The point at which it touches is currently at 1.5 (the location of the derivative).

Therefore, by the slope (or gradient) of the derivative, we must increase w. This is called gradient descent, because we

The curvy line shows the error

function e() as you vary the coefficient w. The straight line is the derivative of the error function at a given w. Notice

During training, the program cannot visualize this graph. All that we can see is one narrow vertical slice, in which

value and the derivative. We move the coefficient in the direction indicated by the derivative and see how much the error improves in the next iteration. In the next iteration, we calculate a new gradient and continue to adjust the coefficient. This same process continues until we can no longer improve the error by a considerable amount.

exist the error at our current coefficient

Chapter Summary

This chapter introduced two forms of linear regression: regular linear regression. Regular linear regression requires that a mostly linear relationship exist between the input vector and output values. Linear regression outputs a single resulting value.

A linear regression algorithm's long-term memory is the coefficients that are used by its equation. These coefficients can be adjusted using the general training algorithms used earlier in this book. However, there a mathematical shortcut that can be employed to quickly determine values

error between the output from the model and the expected outputs contained in the training set.

You will see several such shortcuts through this series. There are general

for the coefficients that minimize the

nearly any type of problem, and there are specialized algorithms that only work with specific models. The special algorithms often use mathematical techniques to perform very efficient optimization of the underlying models.

algorithms that can be used to solve

squares training are two such examples.

This book introduced you to many fundamental algorithms for AI. Subsequent volumes in this series will

Least squares training and reweight least

make use of the fundamental algorithms in this book. While these algorithms are often used as building blocks, they are also very useful in their own right.

build more complex algorithms that

The next book in this series will cover nature inspired algorithms. The only model that we have for true intelligence is the human brain and nature. Because of this, it is natural that we take inspiration from nature to design algorithms. Genetic algorithms, genetic programming, ant colony optimization, particle swarm optimization, and other such algorithms will be explored in the

next book. The next book uses many of the algorithms introduced in this book.

Appendix A Examples

- Downloading Examples
- Structure of Example Download
- Keeping Updated

Artificial Intelligence for Humans

These examples are part of a series of books that is currently under development. Check the above website to see which volumes have been completed and are available. The planned list is shown here.

The following volumes are planned for this series:

- Volume 0: Introduction to the Math of AI
 Volume 1: Fundamental Algorithms
 - Volume 1: Fundamental Algorithms
- Volume 2: Nature Inspired

AlgorithmsVolume 3: Neural Networks

- Volume 4: Support Vector
- Volume 4: Support Vector
 Machines
- Volume 5: Probabilistic Learning

Staying Up to Date

This appendix describes how to obtain the "Artificial Intelligence for Humans" (AIFH) book series examples.

This is probably the most dynamic area of the book. Computer languages are always changing and adding new versions. I will update the examples as this becomes necessary. There are also bugs and corrections. You are encouraged to always make sure you are using the latest version of the book examples.

Because this area is so dynamic, this file may have become out of date. You can always find the latest version of

this file at the following location. https://github.com/jeffheaton/aifh

Obtaining the Examples

This book's examples are provided in a number of computer programming languages. Core example packs are provided for Java, C#, C/C++, Python and R for most volumes. The community may have added other languages as well. All examples can be found at the GitHub repository.

https://github.com/jeffheaton/aifh

You have your choice of two different ways to download the examples.

Download ZIP File

contains all of the example code for the series. A single ZIP file is used to contain all of the examples for the series. Because of this, the contents of this ZIP are frequently updated. If you

are starting a new volume, it is very important that you make sure you have the latest copy. The download can be

you to simply download a ZIP file that

Github provides an icon that allows

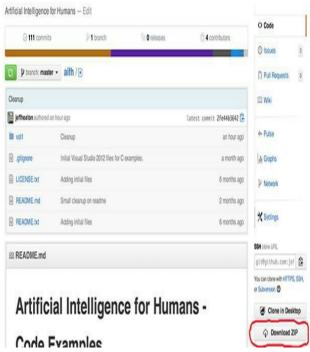
https://github.com/jeffheaton/aifh You can see the download link in

performed from the following URL.

Figure A.1.

Figure A.1: GitHub





Clone the Git Repository

All examples can be obtained using the source control program **git**, if it is installed on your system. The following command clones the examples to your computer. Cloning simply refers to the process of copying the example files.

```
git clone https://github.com/jef:
```

You can also pull the latest updates using the following command.

```
If you would like an introduction to git refer to the following URL.
```

http://git-scm.com/docs/gittutorial

git pull

Example Contents

The entire "Artificial Intelligence for Humans" series is contained in one download. This download is a zip file.

Once you open the examples file you will see the contents see in Figure A.2.

Figure A.2: Examples Download











license used for the book examples. All of the examples for this series are released under the Apache v2.0 license. This is a Free and open-source software (FOSS) license. This means that I do

The license file describes the

retain a copyright to the files. However, you can freely reuse these files in both commercial and non-commercial projects without further permission.

While the book source code is provided free, the book text is not

provided free. These books are commercial products that I sell through a variety of means. You may not redistribute the actual books. This includes the PDF, MOBI, EPUB and any other format the book might be converted

DRM-free form. Your support of this policy is greatly appreciated and does contribute to the future growth of these books.

There are also two README files

included in the download. The

to. I do, however, provide all books in

README.md is a "markdown" file that contains images and formatting. The README.txt file is plane text. Both files contain the same information. For more information on MD files, refer to the following URL.

https://help.github.com/articles/github-

You will find README files at several levels of the examples

flavored-markdown

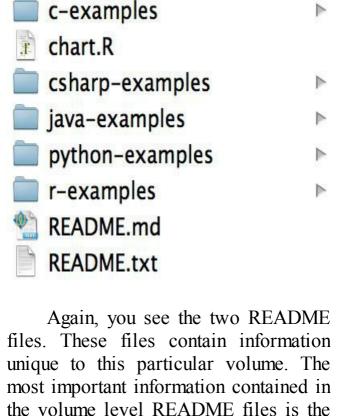
in the examples root (seen above) contains information about the book series.

You will also notice the individual volume folders contained in the

download. The README file contained

download. These are named vol1, vol2, etc. You may not see all of the volumes in the download. Not all of the volumes have been written yet! All of the volumes have the same format. For example, if you were to open Volume 1, you would see the contents listed in Figure A.3.

Figure A.3: Inside Volume 1



packs. This means that some of the example packs may not be complete. The README for the volume will let you know this important information. The volume README also contains the

errata and FAQ for a volume.

current status of the examples. The community often contributes example

You should also see a file named "chart.R". This file contains the source code that I used to create many of the charts in the book. I use the R programming language to produce nearly

all graphs and charts seen in the book. This allows you to see the equations behind the pictures. I do not translate this file to other programming languages. R is simply what I use in the production

like Python, to produce some of the charts, you would see a "chart.py" along with the R code.

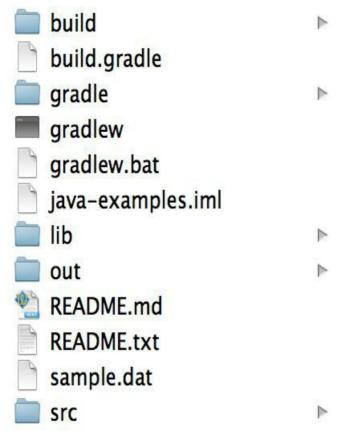
You can see that the above volume contains examples for C, C#, Java,

of the book. If I used another language,

Python and R. These are the core languages that I try to always ensure complete examples for. However, you may see other languages added. Again, always check the README file for the latest information on language translations.

Figure A.4 shows the contents of a typical language pack.

Figure A.4: The Java Language Pack



Notice the README files again? The README files inside of a language folder are VERY important. Inside the above two README files you will find information about using the examples with Java. If you are having trouble using the book's examples with a particular language, the README file should be your first stop. The other files seen above are all unique to Java. The README file above describes these in much greater detail.

Contributing to the Project

Do you want to translate the examples to a new language? Have you found something broken, misspelled, or otherwise botched? You probably have. Fork the project and push a commit revision to GitHub. You will be credited among the growing number of contributors.

The process begins with a fork. You create an account on GitHub and fork the AIFH project. This creates a new project, with a copy of the AIFH files. You will then clone your new for, in a similar way as was described for cloning the main AIFH repositiory. Once

"pull request". Once I get this request I will evaluate your changes/additions and merge it with the main project.

A much more detailed article on

you make your changes you submit a

contributing through GitHub can be found here.

https://help.github.com/articles/fork-a-

nttps://neip.github.com/articles/fork-a-repo

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